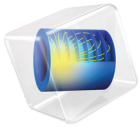

CFD Module

User's Guide

6.3

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CFD Module User's Guide

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1

Introduction

This guide describes the CFD Module, an optional add-on package for COMSOL Multiphysics® that provides you with tools for computational fluid dynamics, CFD. The modeling of fluid flow is an increasingly important part in development of new equipment and processes.

This chapter introduces you to the capabilities of the module. A summary of the physics interfaces and where you can find documentation and model examples is also included. The last section is a brief overview with links to each chapter in this guide.

- About the CFD Module
- Overview of the User's Guide

About the CFD Module

In this section:

- Why CFD Is Important for Modeling
- How the CFD Module Helps Improve Your Modeling
- Where Do I Access the Documentation and Application Libraries?

Why CFD Is Important for Modeling

Computational fluid dynamics, CFD, is an integral part in a constantly growing number of development processes, and is a well established field within many different engineering disciplines; mechanical, chemical, civil, aeronautical, and also in more specialized areas such as biomedical engineering.

Often the flow itself is not the main focus in a simulation. Instead it is how the flow affects other process and application parameters that is important. The transport of species through the different parts of a chemical reactor, the effective cooling of a computer's hard drive and electronics, the dispersion of energy within the damping film of an accelerometer, the extent of nuclear waste spreading from a subterranean repository — all of these are applications for which the flow must be fully understood and is an integral part of the process's description and simulation.

In many situations, while the flow can add necessary operational parameters to a process or application, it is also affected by them. For example, a chemical reactor creates a pressure which disturbs the flow, the electronic heat affects the fluid's density and flow properties, the accelerometer elasticity imposes an oscillation on the flow, while the subterranean environment's poroelasticity changes the course of the flow.

A description combining several physics fields is often required to produce accurate models of real world applications involving fluid flow. Being able to effectively simulate such models increases the understanding of the studied processes and applications, which in turn leads to optimization of the flow and other parameters.

Historically, a sophisticated modeling tool was a privilege that only large companies could afford, for which the savings made in bulk production justified the computer software costs and need for CFD specialists. Today's engineers are educated in the use of software modeling tools, and are often expected to create realistic models of

advanced systems on their personal computers. This is where COMSOL Multiphysics can improve your modeling capabilities.

How the CFD Module Helps Improve Your Modeling

The CFD Module is an optional package that extends the COMSOL Multiphysics modeling environment with customized physics interfaces and functionality optimized for the analysis of all types of fluid flow. It is developed for a wide variety of users including researchers, developers, teachers, and students. It is not just a tool for CFD experts; it can be used by all engineers and scientists who work with systems in which momentum transport through fluid flow is an important part of a process or application.

The module uses the latest research possible to simulate fluid flow and it provides the most user-friendly simulation environment for CFD applications. The solvers and meshes are optimized for fluid-flow applications and have built-in robust stabilization methods.

The readily available coupling of heat and mass transport to fluid flow enables modeling of a wide range of industrial applications such as heat exchangers, turbines, separation units, and ventilation systems.

Ready-to-use interfaces enable you to model laminar and turbulent single- or multiphase flow. Functionality to treat coupled free and porous media flow, stirred vessels, and fluid structure interaction is also included.

Together with COMSOL Multiphysics and its other optional packages, the CFD Module takes flow simulations to a new level, allowing for arbitrary coupling to physics interfaces describing other physical phenomena, such as structural mechanics, electromagnetics, or even user-defined transport equations. This allows for unparalleled modeling capabilities for multiphysics applications involving fluid flow.

Like all COMSOL modules, the interfaces described in this guide include all the steps available for the modeling process, which are described in detail in the *COMSOL Multiphysics Reference Manual*:

- *Definitions* of parameters and component variables
- Creating, importing, and manipulating the *geometry*
- Specifying the *materials* to include in the component
- Defining the *physics* of the fluid flow in domains and on boundaries, and coupling it to other physics

- Set up an appropriate *mesh* for the modeling domain with consideration given to the fluid-flow system's behavior
- Solving the equations that describe a system for stationary or dynamic behavior, or as a parametric or optimization *study*
- Collecting and analyzing *results* to present for further use in other analyses.

Once a model is defined, you can go back and make changes in all of the branches listed, while maintaining consistency in the other definitions throughout. You can restart the solver, for example, using the existing solution as an initial guess or even alter the geometry, while the equations and boundary conditions are kept consistent through the associative geometry feature.

Where Do I Access the Documentation and Application Libraries?

A number of online resources have more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or context-based) help, and the Application Libraries are all accessed through the COMSOL Desktop.

If you are reading the documentation as a PDF file on your computer, the blue links do not work to open an application or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to open other modules, application examples, and documentation sets.

THE DOCUMENTATION AND ONLINE HELP

The *COMSOL Multiphysics Reference Manual* describes the core physics interfaces and functionality included with the COMSOL Multiphysics license. This book also has instructions on how to use COMSOL Multiphysics and how to access the electronic Documentation and Help content.

Opening Topic-Based Help

The Help window is useful as it is connected to the features in the COMSOL Desktop. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then

displays information about that feature (or click a node in the Model Builder followed by the **Help** button (?). This is called *topic-based* (or *context) help*.

Win

To open the **Help** window:

- In the **Model Builder**, **Application Builder**, or **Physics Builder**, click a node or window and then press F1.
- On any toolbar (for example, **Home**, **Definitions**, or **Geometry**), hover the mouse over a button (for example, **Add Physics** or **Build All**) and then press F1.
- From the **File** menu, click **Help** (?).
- In the upper-right corner of the COMSOL Desktop, click the **Help** (?) button.

Mac

Linux

To open the **Help** window:

- In the **Model Builder** or **Physics Builder**, click a node or window and then press F1.
- In the main toolbar, click the **Help** (?) button.
- From the main menu, select **Help>Help**.

Opening the Documentation Window

Mac

Linux

To open the **Documentation** window:

- Press Ctrl+F1.
- In the main toolbar, click the **Documentation** ( ) button.
- From the main menu, select **Help>Documentation**.

THE APPLICATION LIBRARIES WINDOW

Each model or application includes documentation with the theoretical background and step-by-step instructions to create a model or application. The models and applications are available in COMSOL Multiphysics as MPH-files that you can open for further investigation. You can use the step-by-step instructions and the actual models as templates for your own modeling. In most models, SI units are used to describe the relevant properties, parameters, and dimensions, but other unit systems are available.

Once the Application Libraries window is opened, you can search by name or browse under a module folder name. Click to view a summary of the model or application and its properties, including options to open it or its associated PDF document.

Opening the Application Libraries Window

To open the **Application Libraries** window ( ):

CONTACTING COMSOL BY EMAIL

For general product information, contact COMSOL at info@comsol.com.

COMSOL ACCESS AND TECHNICAL SUPPORT

To receive technical support from COMSOL for the COMSOL products, please contact your local COMSOL representative or send your questions to support@comsol.com. An automatic notification and a case number will be sent to you by email. You can also access technical support, software updates, license information, and other resources by registering for a COMSOL Access account.

COMSOL ONLINE RESOURCES

COMSOL website	www.comsol.com
Contact COMSOL	www.comsol.com/contact
COMSOL Access	www.comsol.com/access
Support Center	www.comsol.com/support
Product Download	www.comsol.com/product-download
Product Updates	www.comsol.com/product-update
COMSOL Blog	www.comsol.com/blogs
Discussion Forum	www.comsol.com/forum
Events	www.comsol.com/events
COMSOL Application Gallery	www.comsol.com/models
COMSOL Video Gallery	www.comsol.com/videos
Learning Center	www.comsol.com/support/learning-center
Support Knowledge Base	www.comsol.com/support/knowledgebase

Overview of the User's Guide

The *CFD Module User's Guide* gets you started with modeling CFD systems using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions on how to use COMSOL in general are included with the *COMSOL Multiphysics Reference Manual*. For theory relating to the physics interfaces, see the end of each chapter.

As detailed in the section Where Do I Access the Documentation and Application Libraries? this information can also be searched from the COMSOL Multiphysics software **Help** menu.

TABLE OF CONTENTS, GLOSSARY, AND INDEX

To help you navigate through this guide, see the Contents, Glossary, and Index.

QUICK START GUIDE

The Quick Start Guide includes some basic modeling strategies to get you started modeling fluid flow in your particular application area. For example, it gives some tips about how to control your material properties and how to set the optimal mesh to make solving the model easier and quicker. It also includes a summary of all the physics interfaces included with the CFD Module.

THE PHYSICS INTERFACES

The CFD Module both extends physics interfaces available with COMSOL Multiphysics and provides additional physics interfaces. As a result, the module contains a wide range of physics interfaces for modeling various types of momentum transport. You can simulate laminar and turbulent flow, Newtonian and non-Newtonian flow, isothermal and nonisothermal flow, multiphase flow, and flow in porous media. The CFD Module also provides interfaces for modeling flows that occur in thin-films or in bounded regions, and in stationary and rotating domains.

On top of this, the CFD Module includes physics interfaces for modeling heat transfer, and transport and reactions of chemical species. These are typical phenomena that occur in fluid flow and are strongly coupled to the flow field.

Single-Phase Flow

The Single-Phase Flow Interfaces chapter describes the many physics interfaces available for laminar and turbulent flow. Modeling Single-Phase Flow helps you choose the best Fluid Flow interface for your particular application.

Multiphase Flow

The Multiphase Flow Interfaces chapter describes physics interfaces to model flows with more than one phase, for example flows with two fluids or flows with dispersed droplets or particles. To help you select which physics interface to use see Modeling Multiphase Flow.

Porous Media and Subsurface Flow

The Porous Media and Subsurface Flow Interfaces chapter describes physics interfaces to model flow through porous media, for example groundwater flow or flows through packed bed reactors. To help you select which physics interface to use see Modeling Porous Media and Subsurface Flow.

Heat Transfer and Nonisothermal Flow

The CFD Module includes physics interfaces for the simulation of heat transfer in fluid flow. As with all other physics models simulated in COMSOL Multiphysics, any description involving heat transfer can be directly coupled to any other physical process. This is particularly relevant for systems with fluid flow and mass transfer. The interfaces also allow you to account for heat sources and sinks, such as energy evolving from chemical reactions.

The Heat Transfer and Nonisothermal Flow Interfaces chapter describes these physics interfaces in greater detail. To help you select which physics interface to use see Modeling Heat Transfer in the CFD Module.

High Mach Number Flow

The High Mach Number Flow Interfaces chapter describes three versions of the same predefined multiphysics interface used to model laminar and turbulent compressible flows at high Mach numbers.

Thin-Film Flow

The Thin-Film Flow Interfaces chapter describes physics interfaces that model flow in thin regions such as lubrication shells and fluid bearings.

Shallow Water Equations

The Shallow Water Interface chapter describes a depth-averaged formulation for modeling free-surface flows.

Chemical Species Transport

The Chemical Species Transport Interfaces chapter describes physics interfaces that are used for the simulation of chemical reactions, and mass or material transport through diffusion and convection. Modeling Chemical Species Transport helps you select the best physics interface to use.

The Mathematics Interfaces

Mathematics, Moving Interface Branch describes the **Phase Field** and **Level Set** interfaces found under the **Mathematics** > **Moving Interface** branch. In the CFD Module these physics features are integrated into the relevant physics interfaces.

2

Quick Start Guide

This chapter has some basic modeling strategies to get you started modeling fluid flow in your application area.

In this chapter:

- Modeling and Simulations of Fluid Flow

Modeling and Simulations of Fluid Flow

In this section:

- Modeling Strategy
- Geometric Complexities
- Material Properties
- Defining the Physics Interfaces and Features
- Meshing
- The Choice of Solver and Solver Settings
- The CFD Module Physics Interface Guide
- Common Physics Interface and Feature Settings and Nodes
- The Liquids and Gases Materials Database

The Physics Interfaces and Building a COMSOL Multiphysics Model in the *COMSOL Multiphysics Reference Manual*

Modeling Strategy

Modeling and simulating fluid flow is a cost-effective way for engineers and scientists to understand, develop, optimize, and control designs and processes.

One of the most important things to consider before setting up a model is the accuracy that is required in the simulation results. This determines the level of complexity in the model.

Since fluid flow simulations are often computationally demanding, a multistage modeling strategy is usually required. This implies using a simplified model as a starting point in the project. Complexities can then be introduced gradually so that the effect of each refinement of the model description is well understood before introducing new complexities.

Complexities in the modeling process can be introduced at different stages in order to achieve the desired accuracy. They can be introduced in the description of the

geometry, the physical properties, and in the governing equations. The Model Builder, which shows the sequence of operations in the model tree, is designed with this strategy in mind.

In addition to fluid flow, COMSOL Multiphysics and the CFD Module have predefined multiphysics couplings for fluid flow and other phenomena. Examples of these couplings are heat transfer for free convection and transport of chemical species in simulations of reacting flows. You can also set up your own couplings by defining mathematical expressions of the dependent variables (velocity, pressure, temperature, and so forth) in the physics interfaces for arbitrary multiphysics combinations.

Geometric Complexities

A complicated 3D CAD drawing is usually not the best starting point for the modeling process. A 2D representation of a cross section of the geometry can give valuable initial estimates of the flow field that can be used when setting up the full 3D model. For example, you might be able to determine the pressure variations and the nature of the flow, or whether or not a turbulence model is needed. This provides information about where in the final geometry the most amount of "change" occurs, if a more advanced fluid-flow model or better resolution is required, and what parts of the modeling process are more sensitive than others.

Simplifying the geometry reduces the simulation time. Making use of symmetry planes can cut down the geometry to one half or even less of the original size. Rounding-off corners is another way to reduce mesh resolution. Resolving small geometric parts requires a fine mesh, but the parts themselves can have a negligible effects on the fluid field as a whole.

Geometry Modeling and CAD Tools in the *COMSOL Multiphysics Reference Manual*

Material Properties

Depending on the accuracy required in a simulation, the effort put in acquiring data for the fluid properties can also vary. In many cases, the dependencies of the fluid properties on pressure and temperature have to be taken into account.

For a pressure-driven flow, it is usually a good approach to first set up a model using constant density and viscosity, to get a first estimate of the flow and pressure fields.

Once the model works with constant properties it can be extended by adding the accurate expressions for density and viscosity.

For free convection the density variations drive the flow. The fluid properties' dependencies on the modeled variables, for example temperature, then have to be accounted for from the beginning. In difficult cases, with large temperature variations, it can be beneficial to run a time-dependent simulation even if the purpose of the simulation is to get the results at steady state.

Defining the Physics Interfaces and Features

The CFD Module has physics interfaces for laminar and turbulent single-phase flow, multiphase flow, nonisothermal flow, high Mach number flow, thin-film flow, and porous media flow.

The choice of physics interface and features depends on the accuracy required in a simulation. A fluid that is weakly compressible could be approximated as incompressible if the required accuracy allows for it. A complex turbulence model can be replaced by a much simpler one, again if the resulting accuracy is sufficient. A first step to set up the physics is to start by making the model as simple as possible. The results from such a simulation can reveal useful pieces of information that help later when more complex steps are added to the physics.

The Fluid Flow interfaces can also be coupled to any other physics interface in a multiphysics model. When setting up such a complex multiphysics component involving fluid flow and other coupled physics, it is a good strategy to first define and solve one physics interface at a time. This allows for verification of the model setup, for example to check if the intended domain and boundary settings are reflected in the solution of each decoupled physics interface. The alternative, to debug the model setup with several coupled physics interfaces, can be time consuming.

In steady-state multiphysics simulations, it can also be a good strategy to start by solving the model for each physics interface in a decoupled setup. The solutions from the decoupled models can then be used as initial guesses for the fully coupled model. This is especially recommended for highly nonlinear models. The Study node is designed for this modeling strategy.

Building a COMSOL Multiphysics Model and Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Meshing

The mesh used in a fluid-flow simulation depends on the fluid-flow model and on the accuracy required in the simulation. A fluid-flow model can inherently require a fine resolution in order to converge, even though the results might not require a correspondingly high accuracy. In such cases, it can be a good idea to change the fluid flow model. An example is the low-Reynolds number k-ε model which gives a very accurate description of the flow near solid walls, but requires a very fine mesh there. In many cases, the standard k-ε model with wall functions can deliver an accurate enough result at a much lower computational cost. In other cases, the requirement of accuracy in the results can limit the maximum element size.

There are a number of different mesh types and meshing strategies for fluid flow modeling in COMSOL Multiphysics.

UNSTRUCTURED MESHES

Unstructured meshing is the most general way of creating a mesh and can be used for all types of geometries. The mesh-generating algorithms are highly automated, often creating a good quality mesh from minimal user input. This mesh type is therefore a good choice when the geometry of the domain is evident but the behavior of the mathematical model in it is unknown. Yet, unstructured meshes tend to be isotropic or homogeneous in nature, so that they fail to take advantage of the different resolution requirements in the streamwise and cross-stream directions.

STRUCTURED MESHES

In many ways, the properties of structured meshes complement those of the unstructured type. Structured meshes provide high quality meshes with few elements for sufficiently simple geometries. The properties of a structured mesh can furthermore be used to create very efficient numerical methods. Finally, it is often easier to control the mesh when high *anisotropy* or large variations in mesh size and distribution is required, as the size of a structured mesh can be easily increased linearly or geometrically with the dimensions of the computational domain.

SWEPT MESHES

Swept meshes are a particular form of structured meshes, sometimes denoted semistructured. These are generated in 3D by creating a mesh at a source face and then sweeping it along the domain to a destination face, such as from a cut in the cylindrical part of a polymerization reactor to its outlet face. A swept mesh is structured in the sweep direction, while the mesh at the source and destination faces can be either

structured or unstructured. As is the case for structured meshes, the model geometry determines if a swept mesh is applicable. Swept meshes are typically ideal when the cross section in the sweep direction is constant, which is the case for channels and pipes, for example. Revolving a mesh around a symmetry axis is another useful sweep operation.

BOUNDARY LAYER MESHES

A boundary layer mesh is a mesh with an element distribution that is stacked or dense in the direction normal to a boundary. It is created by inserting structured layers of elements along specific boundaries and merging the outer layer with the surrounding structured or unstructured mesh. This type of mesh is useful for many fluid flow applications especially when coupled to mass and energy transfer, where thin *boundary layers* need to be resolved. This is also the default physics-induced mesh for fluid flow.

MESH CONVERGENCE

Ideally, a mesh convergence analysis should be performed in order to estimate the accuracy of a simulation. This means that the mesh should be made twice as fine in each spatial direction and the simulation carried out once again on the refined mesh. If the change in critical solution parameters for the original mesh and the finer mesh is within the required tolerance, the solution can be regarded as being mesh-converged. For practical reasons, it is seldom possible to make the mesh twice as fine in each direction. Instead, some critical regions can be identified and the mesh is refined only there.

Meshing in the *COMSOL Multiphysics Reference Manual*

The Choice of Solver and Solver Settings

The default solver for the Fluid Flow interfaces is optimized for a large variety of fluid flow conditions and applications. The suggested solver depends on the physics interface and the study type.

The default solver settings is a tradeoff between performance and robustness. The more advanced the model, the more the solver can need tuning to obtain a solution. This is another reason why it is good to start with a reduced model description rather than the complete description.

2D models and small 3D models get so-called direct-solver suggestions. Direct solvers are robust but the memory requirement scales somewhere between $N^{1.5}$ and N^2 where

N is the number of degrees of freedom in the model. This means that a direct solver becomes prohibitively expensive for large problems. Large 3D models therefore get iterative solver suggestions per default. The memory requirement for an iterative solver optimally scales as N. The drawback with iterative solvers is that they are less robust than direct solvers. A model can converge with a direct solver but fail with an iterative solver. Large models therefore require more care when being set up than small models do.

For well-posed models, there are possibilities to tune the default solvers to gain performance. This is especially true for time-dependent models with a variety of solver settings providing options to reduce the computational time.

Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

The CFD Module Physics Interface Guide

The CFD Module extends the functionality of the physics interfaces of the base package for COMSOL Multiphysics. The details of the physics interfaces and study types for the CFD Module are listed in the table. The functionality of the COMSOL Multiphysics base package is listed in the *COMSOL Multiphysics Reference Manual*.

In the *COMSOL Multiphysics Reference Manual:*

- Studies and Solvers
- The Physics Interfaces
- For a list of all the core physics interfaces included with a COMSOL Multiphysics license, see Physics Interface Guide.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Chemical Species Transport				
Transport of Diluted Species[1]		tds	all dimensions	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Transport of Concentrated Species		tcs	all dimensions	stationary; time dependent
Transport of Diluted Species in Porous Media		tds	all dimensions	stationary; time dependent
Transport of Concentrated Species in Porous Media		tcs	all dimensions	stationary; time dependent
Reacting Flow				
Laminar Flow, Diluted Species[1]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow, Concentrated Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, Diluted Species				
Turbulent Flow, k-ε		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, SST		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Low Re k-ε		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Concentrated Species				
Turbulent Flow, k-ε		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω		—	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, SST		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Low Re k-ε		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Reacting Flow in Porous Media				
Transport of Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
High Mach Number Reacting Flow				
Laminar Flow[3]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow, Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow[3]				
Turbulent Flow, k-ε[3]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, Spalart–Allmaras[3]		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Diluted Species				
Turbulent Flow, k-ε		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, Spalart–Allmaras		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Dispersed Two-Phase Flow with Species Transport				
Laminar Flow		—	3D, 2D,	stationary; time dependent
Turbulent Flow				
Turbulent Flow, k-ε		—	3D, 2D	stationary; time dependent
Turbulent Flow, k-ω		—	3D, 2D	stationary; time dependent
Turbulent Flow, SST		—	3D, 2D	stationary with initialization; time dependent with initialization
Turbulent Flow, Low Re k-ε		—	3D, 2D	stationary with initialization; time dependent with initialization
Vapor-Liquid Equilibrium				
Laminar Vapor Flow(3)		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Two-Phase Flow(3)		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Vapor Flow				
Turbulent Flow, k-ε(3)		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω(3)		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, SST(3)		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, Low Re k-ε[3]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Fluid Flow				
Single-Phase Flow				
Creeping Flow		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow[1]		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Viscoelastic Flow		vef	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow				
Turbulent Flow, Algebraic yPlus		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, L-VEL		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, k-ε		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, Realizable k-ε		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k-ω		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, SST		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, Low Re k-ε		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Spalart–Allmaras		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, v2-f		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Wilcox R-ω		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, SSG-LRR		spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Large Eddy Simulation				
LES RBVM		spf	3D	time dependent
LES RBVMWV		spf	3D	time dependent
LES Smagorinsky		spf	3D	time dependent
Detached Eddy Simulation				
DES RBVM, Spalart–Allmaras		spf	3D	time dependent
DES RBVMWV, Spalart–Allmaras		spf	3D	time dependent
DES Smagorinsky, Spalart–Allmaras		spf	3D	time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Rotating Machinery, Fluid Flow				
Rotating Machinery, Laminar Flow		spf	3D, 2D	frozen rotor; time dependent
Rotating Machinery, Turbulent Flow, Algebraic yPlus		spf	3D, 2D	frozen rotor with initialization; time dependent with initialization
Rotating Machinery, Turbulent Flow, L-VEL		spf	3D, 2D	frozen rotor with initialization; time dependent with initialization
Rotating Machinery, Turbulent Flow, k-ε		spf	3D, 2D	frozen rotor; time dependent
Potential Flow				
Incompressible Potential Flow		ipf	3D, 2D, 2D axisymmetric	stationary
Compressible Potential Flow		cpf	all dimensions	stationary; time dependent
Multiphase Flow				
Bubbly Flow				
Laminar Bubbly Flow		bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Bubbly Flow, Turbulent Flow				
Bubbly Flow, Algebraic yPlus		bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, L-VEL		bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Bubbly Flow, k-ε		bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Bubbly Flow, Realizable k-ε		bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Bubbly Flow, k-ω		bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Bubbly Flow, SST		bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, Low Re k-ε		bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, Spalart–Allmaras		bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, v2-f		bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model				
Mixture Model, Laminar Flow		mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, Turbulent Flow				
Mixture Model, Algebraic yPlus		mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, L-VEL		mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Mixture Model, k-ε		mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, Realizable k-ε		mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, k-ω		mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, SST		mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, Low Re k-ε		mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, Spalart–Allmaras		mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, v2-f		mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Euler–Euler Model				
Euler–Euler Model, Laminar Flow		ee	3D, 2D, 2D axisymmetric	stationary; time dependent
Euler–Euler Model, Turbulent Flow		ee	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport Mixture Model				
Phase Transport, Mixture Model, Laminar Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport, Mixture Model, Algebraic yPlus		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Phase Transport, Mixture Model, L-VEL		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, k-ε		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport, Mixture Model, Realizable k-ε		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport, Mixture Model, k-ω		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport, Mixture Model, SST		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, Low Re k-ε		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, Spalart–Allmaras		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, v2-f		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model				
Nonisothermal Mixture Model, Laminar Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Mixture Model, Algebraic yPlus		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Nonisothermal Mixture Model, L-VEL		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, k-ε		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Mixture Model, Realizable k-ε		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Mixture Model, k-ω		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Mixture Model, SST		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, Low Re k-ε		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, Spalart–Allmaras		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, v2-f		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Two-Phase Flow, Moving Mesh				
Laminar Two-Phase Flow, Moving Mesh		—	3D, 2D, 2D axisymmetric	time dependent
Two-Phase Flow, Level Set				
Laminar Two-Phase Flow, Level Set		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Level Set, Algebraic yPlus		—	3D, 2D, 2D axisymmetric	time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Two-Phase Flow, Level Set, L-VEL		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Level Set, k-ε		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Level Set, Realizable k-ε		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Level Set, k-ω		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Level Set, SST		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Level Set, Low Re k-ε		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Level Set, Spalart–Allmaras		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Level Set, v2-f		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field				
Laminar Two-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Phase Field, Algebraic yPlus		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field, L-VEL		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field, k-ε		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Phase Field, Realizable k-ε		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Phase Field, k-ω		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Phase Field, SST		—	3D, 2D, 2D axisymmetric	time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Two-Phase Flow, Phase Field, Low Re k-ε		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field, Spalart–Allmaras		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field, v2-f		—	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Thin-Film Flow, Phase Field				
Two-Phase Thin-Film Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Three-Phase Flow, Phase Field				
Laminar, Three-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Phase Transport				
Phase Transport		phtr	all dimensions	stationary; time dependent
Phase Transport in Porous Media		phtr	all dimensions	stationary; time dependent
Phase Transport in Free and Porous Media Flow		phtr	all dimensions	stationary; time dependent
Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent
Multiphase Flow in Porous Media		—	all dimensions	stationary; time dependent
Multiphase Free and Porous Media Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Two-Phase Darcy's Law		tpdl	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Brinkman		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Darcy		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Thin-Film and Porous Media Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent; frequency domain
Nonisothermal Flow				
Laminar Flow[1,2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Brinkman Equations		—	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF
Viscoelastic Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow				
Turbulent Flow, Algebraic yPlus[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, L-VEL[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Realizable k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, k-ω[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, SST[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Low Re k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Spalart–Allmaras[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, v2-f[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Large Eddy Simulation				
LES RBVM		—	3D	time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
LES RBVMWV		—	3D	time dependent
LES Smagorinsky		—	3D	time dependent
Rotating Machinery, Nonisothermal Flow				
Laminar Flow		—	3D, 2D	frozen rotor; time dependent
High Mach Number Flow				
High Mach Number Flow, Laminar		hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent
High Mach Number Flow, Algebraic yPlus		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
High Mach Number Flow, L–VEL		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
High Mach Number Flow, Spalart–Allmaras		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
High Mach Number Flow, k-ε		hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent
High Mach Number Flow, Realizable k-ε		hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent
High Mach Number Flow, k-ω		hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent
High Mach Number Flow, SST		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
High Mach Number Flow, Low Reynolds Number k-ε		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
High Mach Number Flow, v2-f		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
High Mach Number Flow, Wilcox R-ω		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
High Mach Number Flow, SSG-LRR		hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Compressible Euler Equations		cee	3D, 2D	time dependent
Rotating Machinery, High Mach Number Flow				
High Mach Number Flow, Laminar		—	3D, 2D	frozen rotor; time dependent
High Mach Number Flow, k-ε		—	3D, 2D	frozen rotor; time dependent
High Mach Number Flow, Spalart–Allmaras		—	3D, 2D	frozen rotor with initialization; time dependent with initialization
Fluid-Structure Interaction				
Fluid–Solid Interaction, Fixed Geometry[2]		—	3D, 2D, 2D axisymmetric	stationary; stationary, one way; time dependent; time dependent, one way
Fluid–Solid Interaction, Two-Phase Flow, Phase Field, Fixed Geometry[2]		—	3D, 2D, 2D axisymmetric	time dependent; time dependent with phase initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Solid–Thin-Film Damping[2]		—	3D, 2D, 2D axisymmetric	stationary; eigenfrequency; time dependent; t frequency domain;
Thin-Film Flow				
Thin–Film Flow		tff	3D, 2D, 2D axisymmetric	stationary; time dependent; frequency domain; eigenfrequency
Thin–Film Flow, Domain		tff	2D	stationary; time dependent; frequency domain; eigenfrequency
Shallow Water Equations				
Shallow Water Equations, Time Explicit		swe	1D and 2D	time dependent
Heat Transfer				
Heat Transfer in Fluids[1]		ht	all dimensions	stationary; time dependent
Heat Transfer in Solids and Fluids[1]		ht	all dimensions	stationary; time dependent
Conjugate Heat Transfer				
Laminar Flow[(1,2)]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow				
Turbulent Flow, Algebraic yPlus[(2)]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, L-VEL[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Realizable k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, k-ω[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, SST[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Low Re k-ε[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Spalart–Allmaras[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, v2-f[2]		—	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Heat Transfer in Porous Media		ht	all dimensions	stationary; time dependent
Structural Mechanics				
Mathematics				
Moving Interface				
Level Set		ls	all dimensions	time dependent with phase initialization
Level Set in Porous Media		ls	all dimensions	time dependent with phase initialization
Phase Field in Fluids		pf	all dimensions	time dependent; time dependent with phase initialization
Phase Field Thin-Film Flow		pftff	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Ternary Phase Field		terpf	3D, 2D, 2D axisymmetric	time dependent

[1] This physics interface is included with the core COMSOL package but has added functionality for this module.

[2] This physics interface is a predefined multiphysics coupling that automatically adds all the physics interfaces and coupling features required.

[3] Requires the addition of the Chemical Reaction Engineering Module

Common Physics Interface and Feature Settings and Nodes

There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in

the same way no matter the physics interface or feature being used. There are also some physics feature nodes that display in COMSOL Multiphysics.

In each module's documentation, only unique or extra information is included; standard information and procedures are centralized in the *COMSOL Multiphysics Reference Manual*.

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Liquids and Gases Materials Database

The CFD Module includes an additional **Liquids and Gases** material database with temperature-dependent fluid properties.

For detailed information about materials and the Liquids and Gases Material Library, see Materials in the *COMSOL Multiphysics Reference Manual*.

3

Single-Phase Flow Interfaces

There are several fluid flow physics interfaces available as listed in The CFD Module Physics Interface Guide. This chapter describes the physics interfaces found under the **Fluid Flow** > **Single-Phase Flow** branch ( ). The section Modeling Single-Phase Flow helps to choose the best physics interface to start with.

In this chapter:

- The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces
- The Rotating Machinery, Laminar and Turbulent Flow Interfaces
- The Viscoelastic Flow Interface
- The Potential Flow Interfaces
- Theory for the Single-Phase Flow Interfaces
- Theory for the Turbulent Flow Interfaces
- Theory for the Large Eddy Simulation Interfaces
- Theory for the Detached Eddy Simulation Interfaces
- Theory for the Rotating Machinery Interfaces
- Theory for the Viscoelastic Flow Interface

- Theory for the Incompressible Potential Flow Interface
- The Wall Distance Interface is also available and described in the *COMSOL Multiphysics Reference Manual* including the theory and how it relates to fluid flow.

Modeling Single-Phase Flow

The descriptions in this section are structured based on the order displayed in the **Fluid Flow** branch. All the physics interfaces described in this section are found under the **Fluid Flow** > **Single-Phase Flow** branch ( ). Because most of the physics interfaces are integrated with each other, many physics features described cross reference to other physics interfaces. For example, nodes are usually available in both the laminar flow (Creeping Flow and Laminar Flow) and turbulent flow (Algebraic yPlus, L-VEL, k-ε, k-ω, SST, low Reynolds number k-ε, Spalart–Allmaras, and v2-f turbulence models) interfaces.

In this section:

- Selecting the Right Physics Interface
- The Single-Phase Flow Interface Options
- Coupling to Other Physics Interfaces

The Wall Distance Interface in the *COMSOL Multiphysics Reference Manual*

Selecting the Right Physics Interface

The Single-Phase Flow branch included with the CFD Module has a number of subbranches with physics interfaces that describe different types of single-phase fluid flow. One or more of these physics interfaces can be added, either singularly or in combination with other physics interfaces for mass transport and heat transfer, for example.

Different types of flow require different equations to describe them. If the type of flow to model is already known, then select it directly. However, when you are uncertain of the flow type, or because it is difficult to reach a solution easily, you can start instead with a simplified model and add complexity as the model is built. Then test your way forward and compare models and results. For single-phase flow, the Laminar Flow interface is a good place to start if this is the case.

In other cases, you may know exactly how a fluid behaves and which equations, models, or physics interfaces best describe it, but because the model is so complex it is difficult to reach an immediate solution. Simpler assumptions may need to be made to

solve the problem, and other physics interfaces might be better to fine-tune the solution process for the more complex problem. The next section gives you an overview of each of the Single-Phase Flow interfaces to help you choose.

The Single-Phase Flow Interface Options

Several of the physics interfaces vary only by one or two default settings (see Table 3-1) in the *Physical Model* and *Turbulence* sections, which are selected either from a checkbox or list. For the Single-Phase Flow branch, all except the Rotating Machinery interfaces have the same *Name* (`spf`). The differences are based on the default settings required to model that type of flow as described in Table 3-1. Figure 3-1 shows the **Settings** window for Laminar Flow where you choose the type of compressibility (incompressible, weakly compressible or compressible at *Mach numbers* below 0.3) and the turbulence type and model (or none for laminar flow), and a checkbox to model Stokes flow by neglecting the inertial term.

TABLE 3-1: THE SINGLE-PHASE FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	TURBULENT MODEL TYPE	LES MODEL/ TURBULENCE MODEL	NEGLECT INERTIAL TERM (STOKES FLOW)
Creeping Flow	spf	Incompressible flow	None	n/a	Stokes Flow
Laminar Flow	spf	Incompressible flow	None	n/a	None
Turbulent Flow, Algebraic yPlus	spf	Incompressible flow	RANS-EVM	Algebraic yPlus	None
Turbulent Flow, L-VEL	spf	Incompressible flow	RANS-EVM	L-VEL	None
Turbulent Flow, k-ε	spf	Incompressible flow	RANS-EVM	k-ε	None
Turbulent Flow, Realizable k-ε	spf	Incompressible flow	RANS-EVM	Realizable k-ε	None
Turbulent Flow, k-ω	spf	Incompressible flow	RANS-EVM	k-ω	None
Turbulent Flow, SST	spf	Incompressible flow	RANS-EVM	SST	None
Turbulent Flow, Low Re k-ε	spf	Incompressible flow	RANS-EVM	Low Reynolds number k-ε	None

TABLE 3-1: THE SINGLE-PHASE FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	TURBULENT MODEL TYPE	LES MODEL/ TURBULENCE MODEL	NEGLECT INERTIAL TERM (STOKES FLOW)
Turbulent Flow, Spalart–Allmaras	spf	Incompressible flow	RANS-EVM	Spalart–Allmaras	None
Turbulent Flow, v2-f	spf	Incompressible flow	RANS-EVM	v2-f	None
Turbulent Flow, Wilcox R-ω	spf	Incompressible flow	RANS-RSM	Wilcox R-ω	None
Turbulent Flow, SSG-LRR	spf	Incompressible flow	RANS-RSM	SSG-LRR	None
LES RBVM	spf	Incompressible flow	LES	RBVM	None
LES RBVMWV	spf	Incompressible flow	LES	RBVMWV	None
LES Smagorinsky	spf	Incompressible flow	LES	Smagorinsky	None
DES RBVM, Spalart–Allmaras	spf	Incompressible flow	DES	RBVM/ Spalart–Allmaras	None
DES RBVMWV, Spalart–Allmaras	spf	Incompressible flow	DES	RBVMWV/ Spalart–Allmaras	None
DES Smagorinsky, Spalart–Allmaras	spf	Incompressible flow	DES	Smagorinsky /Spalart–Allmaras	None
Rotating Machinery, Laminar Flow	spf	Incompressible flow	None	None	None
Rotating Machinery, Turbulent Flow, Algebraic yPlus	spf	Incompressible flow	RANS-EVM	Algebraic yPlus	None
Rotating Machinery, Turbulent Flow, L-VEL	spf	Incompressible flow	RANS-EVM	L-VEL	None
Rotating Machinery, Turbulent Flow, k-ε	spf	Incompressible flow	RANS-EVM	k-ε	None
Viscoelastic Flow	vef	Incompressible flow	n/a	n/a	n/a

TABLE 3-1: THE SINGLE-PHASE FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	TURBULENT MODEL TYPE	LES MODEL/ TURBULENCE MODEL	NEGLECT INERTIAL TERM (STOKES FLOW)
Incompressible Potential Flow	ipf	Incompressible flow	n/a	n/a	n/a
Compressible Potential Flow	cpf	Compressible flow	n/a	n/a	n/a

CREEPING FLOW

The Creeping Flow Interface ( ) models the Navier–Stokes equations without the contribution of the inertia term. This is often referred to as Stokes flow and is appropriate for flow at small Reynolds numbers, such as in very small channels or in microfluidic applications.

The Creeping Flow interface can also be activated by selecting a checkbox in the Laminar Flow interface. This physics interface can also model non-Newtonian fluids, using the predefined non-Newtonian models.

LAMINAR FLOW

The Laminar Flow Interface ( ) is used primarily to model flow at small to intermediate Reynolds numbers. The physics interface solves the Navier–Stokes equations, and by default assumes the flow to be incompressible; that is, the density is assumed to be constant.

Compressible flow is possible to model in this physics interface but you have to maintain control of the density and any of the mass balances that are deployed to accomplish this.

The Laminar Flow Interface allows you to model porous media flow or even mixed free- and porous media flow. A volume force due to gravity can optionally be included.

This physics interface also allows you to simulate flows of the inelastic non-Newtonian fluids. You can model the fluid using the Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models.

You can also describe other material properties such as density by entering equations for its dependence on fluid composition and pressure (for compressible flow), or temperature. Many materials in the material libraries use temperature- and pressure-dependent property values. If the density is affected by temperature, a

nonisothermal flow interface may be applicable (see The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces).

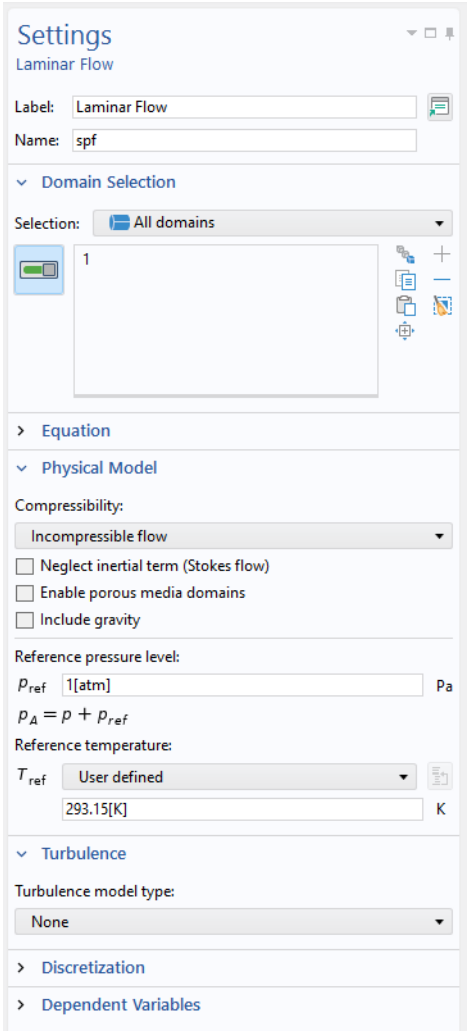


Figure 3-1: The Settings window for the Laminar Flow interface. Model incompressible or compressible flow, laminar or turbulent flow, Stokes flow, and/or porous media flow. Combinations are also possible.

TURBULENT FLOW

The various forms of the Single-Phase Flow, Turbulent Flow interfaces ( ) model flow of large Reynolds numbers. The interfaces solve the Reynolds-averaged Navier–

Stokes (RANS) equations for the averaged velocity field and averaged pressure as well as models for the turbulent viscosity. See The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces for links to the physics interface information.

There are several turbulence models available: two algebraic turbulence models, the Algebraic yPlus and L-VEL models, and nine transport-equation models, including a standard k-ε model, the Realizable k-ε model, a k-ω model, an SST model, a Low Reynolds number k-ε model, the Spalart–Allmaras model, the v2-f model, the Wilcox R-ω model, and the SSG-LRR model. Each model has its merits and weaknesses. See the Theory for the Turbulent Flow Interfaces for more details.

Similarly to the Laminar Flow interface, incompressible flow is selected by default. If required, this can be changed to compressible flow. Non-Newtonian fluid models are not available for the Turbulent Flow interfaces

LARGE EDDY SIMULATION

The Single-Phase Flow, Large Eddy Simulation (LES) interfaces ( ) also model flow at large Reynolds numbers. The LES interfaces are designed for resolving the larger three-dimensional unsteady eddies whereas the effect of the smaller eddies are modeled. Hence, simulations with these interfaces must be three-dimensional and time-dependent.

There are three LES models: the Residual-Based Variational Multiscale (RBVM) model, the Residual-Based Variational Multiscale with Viscosity (RBVMWV) model, and the Smagorinsky model. Of these three, the first two use consistent modeling for the unresolved scales. This means that the modeled stresses in the momentum equation vanish in the limit when all scales are resolved. They can therefore also be used to study laminar or transitional flow.

The current formulations are applicable to flows of Newtonian fluids.

DETACHED EDDY SIMULATION

The Single-Phase Flow, Detached Eddy Simulation (DES) interfaces ( ) resolve the largest three-dimensional turbulent eddies whereas the effect of the smaller eddies are modeled by one of the LES models in the bulk, and by a RANS model near walls. Simulations with these interfaces must be three-dimensional and time-dependent.

There are three DES models: the Residual-Based Variational Multiscale Spalart–Allmaras (DES RBVM, Spalart–Allmaras) model, the Residual-Based Variational

Multiscale with Viscosity Spalart–Allmaras (DES RBVMWV, Spalart–Allmaras) model, and the Smagorinsky, Spalart–Allmaras (DES Smagorinsky, Spalart–Allmaras) model.

The current formulations are applicable to flows of Newtonian fluids.

ROTATING MACHINERY

The Rotating Machinery, Laminar and Turbulent Flow Interfaces ( ) model fluid flow in geometries with rotating parts. For example, stirred tanks, mixers, propellers, and pumps.

When the Rotating Machinery, Fluid Flow interfaces are added using the Model Wizard, a Rotating Domain is added under the Definitions node. These interfaces support compressible, weakly compressible and incompressible flow, the flow of non-Newtonian fluids, as well as turbulence. They also support creeping flow.

THE VISCOELASTIC FLOW INTERFACE

The Viscoelastic Flow Interface ( ) is used for simulating single-phase flows of viscoelastic fluids. The physics interface is only suitable for incompressible flows.

POTENTIAL FLOW

The Potential Flow Interfaces ( ) can be used to model irrotational flow, or to get initial values for other fluid-flow interfaces.

Coupling to Other Physics Interfaces

Often, you may want to simulate applications that couple fluid flow to another type of phenomenon described in another physics interface. Although this is not often another type of flow, it can still involve physics interfaces supported in the CFD Module and in the COMSOL Multiphysics base package. This is often the case for applications that include chemical reactions and mass transport (see Chemical Species Transport Interfaces), or energy transport, found in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of heat transfer, including radiation, can be found in the Heat Transfer Module, while a wider variety of tools for modeling chemical reactions and mass transport are found in the Chemical Reaction Engineering Module. Fluid flow is an important component for cooling electromagnetic phenomena, such as heat created through induction and microwave heating, which are simulated using the AC/DC Module and RF Module, respectively. Many applications involve the effect of fluid-imposed loads on structural applications, for example, fluid-structure interaction

(FSI). The Structural Mechanics Module and MEMS Module have physics interfaces specifically for these multiphysics applications.

You can easily couple a 1D pipe segment modeled with the Pipe Flow interface with a 3D single phase flow using a Pipe Connection multiphysics coupling. This feature is available with a license for the Pipe Flow Module. For details, see the section Pipe Connection in the *Pipe Flow Module User's Guide*.

The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces

In this section:

- The Creeping Flow Interface
- The Laminar Flow Interface
- The Turbulent Flow, Algebraic yPlus Interface
- The Turbulent Flow, L-VEL Interface
- The Turbulent Flow, k-ε Interface
- The Turbulent Flow, Realizable k-ε Interface
- The Turbulent Flow, k-ω Interface
- The Turbulent Flow, SST Interface
- The Turbulent Flow, Low Re k-ε Interface
- The Turbulent Flow, Spalart–Allmaras Interface
- The Turbulent Flow, v2-f Interface
- The Turbulent Flow, Wilcox R-ω Interface
- The Turbulent Flow, SSG-LRR Interface
- The LES RBVM Interface
- The LES RBVMWV Interface
- The LES Smagorinsky Interface
- The DES RBVM, Spalart–Allmaras Interface
- The DES RBVMWV, Spalart–Allmaras Interface

- The DES Smagorinsky, Spalart–Allmaras Interface
- Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

- Theory for the Single-Phase Flow Interfaces

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings** sections, some of them accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Creeping Flow Interface

The **Creeping Flow (spf)** interface ( ) is used for simulating fluid flows at very low Reynolds numbers for which the inertial term in the Navier–Stokes equations can be neglected. Creeping flow, also referred to as Stokes flow, occurs in systems with high viscosity or small geometrical length scales (for example, in microfluidics and MEMS devices). The fluid can be compressible or incompressible, as well as Newtonian or non-Newtonian.

The equations solved by the Creeping Flow interface are the Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Creeping Flow interface can be used for stationary and time-dependent analyses.

The main feature is the **Fluid Properties** node, which adds the Stokes equations and provides an interface for defining the fluid material and its properties. Except where noted below, see The Laminar Flow Interface for all other settings.

PHYSICAL MODEL

By default, the **Neglect inertial term (Stokes flow)** checkbox is selected. If unchecked, or, if the **Turbulence model type** is changed to **RANS-EVM** or **RANS-RSM**, the inertial terms are included in the computations.

DISCRETIZATION

By default, the Creeping Flow interface uses **P2+P1** elements. Contrary to general laminar and turbulent single-phase flow simulations employing purely linear P1+P1 elements, P2+P1 elements are well suited for most creeping flow simulations but are

not in general fully conservative. Full conservation properties and high accuracy is obtained by selecting P2+P2 or P3+P3 elements.

Note that P1+P1, P2+P2, and P3+P3 discretizations (the so-called equal order interpolations) require streamline diffusion to be active.

- The Laminar Flow Interface
- Theory for the Single-Phase Flow Interfaces

The Laminar Flow Interface

The **Laminar Flow (spf)** interface ( ) is used to compute the velocity and pressure fields for the flow of a single-phase fluid in the laminar flow regime. A flow remains laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence. This critical Reynolds number depends on the model, but a classical example is pipe flow, where the critical Reynolds number is known to be approximately 2000.

The physics interface supports incompressible flow, weakly compressible flow (the density depends on temperature but not on pressure), and compressible flow at low Mach numbers (typically less than 0.3). It also supports flow of non-Newtonian fluids.

The equations solved by the Laminar Flow interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Laminar Flow interface can be used for stationary and time-dependent analyses. Time-dependent studies should be used in the high-Reynolds number regime as these flows tend to become inherently unsteady.

When the Laminar Flow interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**. Other nodes that implement, for example, boundary conditions and volume forces, can be added from the **Physics** toolbar or from the context menu displayed when right-clicking **Laminar Flow**.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Physics interface variables can be referred to using the pattern

<name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is spf.

About the Physics Interface Label Names

The label for a single-phase flow interface (the node name in the Model Builder) is dynamic and is reset according to the turbulence model and the neglect inertial term (Stokes flow) property set at the physics interface level. The availability also depends on the software license.

For example, a Laminar Flow interface is added to the Model Tree. If the **Low Reynolds number k-ε** turbulence model is selected, the interface **Label** changes to **Turbulent Flow, Low Re k-ε**, which is the same Label that displays when the corresponding interface is added from the Model Wizard or Add Physics window.

If the **Neglect inertial term (Stokes flow)** checkbox is selected, then the Label changes to **Creeping Flow**, which is the same Label that displays when that interface is added from the Model Wizard or Add Physics window.

PHYSICAL MODEL

Compressibility

Depending of the fluid properties and the flow regime, three options are available for the **Compressibility** option. In general the computational complexity increases from **Incompressible flow** to **Weakly compressible flow** to **Compressible flow (Ma<0.3)** but the underlying hypotheses are increasingly more restrictive in the opposite direction.

When the **Incompressible flow** option (default) is selected, the incompressible form of the Navier–Stokes and continuity equations is applied. In addition, the fluid density is evaluated at the **Reference pressure level** defined in this section. The **Reference temperature** is set to 293.15 K.

The **Weakly compressible flow** option models compressible flow when the pressure dependency of the density can be neglected. When selected, the compressible form of the Navier–Stokes and continuity equations is applied. In addition, the fluid density is evaluated at the **Reference pressure level** defined in this section.

When the **Compressible flow (Ma<0.3)** option is selected, the compressible form of the Navier–Stokes and continuity equations is applied. $\mathrm{Ma} < 0.3$ indicates that the inlet and outlet conditions, as well as the stabilization, may not be suitable for transonic and supersonic flow. For more information, see The Mach Number Limit.

Swirl Flow

The velocity component, u_φ, in the azimuthal direction can be included for 2D axisymmetric components by selecting the **Swirl flow** checkbox. While u_φ can be nonzero, there can be no gradients in the φ direction. Also see General Single-Phase Flow Theory.

Neglect Inertial Term (Stokes Flow)

For low Reynolds number flows, the inertial terms in the Navier–Stokes equations may be neglected.

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** checkbox is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. The **Fluid and Matrix Properties** can be applied on all domains or on a subset of the domains.

Porous Treatment of No Slip Condition

Porous treatment of no slip condition is available when **Enable porous media domains** is activated. It controls how the **No Slip** condition on **Wall** boundaries and **Interior Wall** boundaries adjacent to **Porous Medium** should be treated. The options are **Standard no slip formulation** (default) and **Porous slip**. The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall.

Include Gravity

When the **Include gravity** checkbox is selected, a global **Gravity** feature is shown in the interface model tree, and the buoyancy force is included in the Navier–Stokes equations.

Also, when the **Include gravity** checkbox is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes

are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Natural convection is induced by variations in magnitude of the buoyancy force that is defined from the density. For incompressible flow, the density is constant; hence the buoyancy force is homogeneous and natural convection cannot be modeled. Nevertheless, using the **Nonisothermal Flow** multiphysics coupling, the buoyancy force is defined using the thermal expansion coefficient and the temperature. Hence, in this case natural convection is accounted for, following the Boussinesq approximation.

Use Shallow Channel Approximation

For 2D components, selecting the **Use shallow channel approximation** checkbox enables modeling of fluid flow in shallow channels in microfluidics applications. Such channels often have an almost rectangular cross section where the **Channel thickness** d_z is much smaller than the channel width. Simple 2D components often fail to give correct results for this type of problems because they exclude the boundaries that have the greatest effect on the flow. The shallow channel approximation takes the effect of these boundaries into account by adding a drag term as a volume force to the momentum equation. The form of this term is

$$\mathbf{F}_\mu = -12\frac{\mu \mathbf{u}}{d_z^2} \tag{3-1}$$

where μ is the fluid's dynamic viscosity, $\mathbf{u}$ is the velocity field, and d_z is the channel thickness. This term represents the resistance that the parallel boundaries impose on the flow; however, it does not account for any changes in velocity due to variations in the cross-sectional area of the channel.

Reference Values

Reference values are global quantities used to evaluate the density of the fluid when the **Incompressible flow** or the **Weakly compressible flow** option is selected and to define the gravity force.

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{\text{ref}}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure

whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the reference density.

Reference temperature The reference temperature is used to define the reference density.

Reference position When **Include gravity** is selected, the reference position can be defined. It corresponds to the location where the total pressure (that includes the hydrostatic pressure) is equal to the **Reference pressure level**.

TURBULENCE

Turbulence Model Type

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM** (Reynolds-Averaged Navier–Stokes, eddy-viscosity model), **RANS-RSM** (Reynolds-Averaged Navier–Stokes, Reynolds stress model), or to **LES** (Large Eddy Simulation).

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field** $\mathbf{u}$ and its components, and the **Pressure** p.

If required, the names of the field, component, and dependent variable can be edited. Editing the name of a scalar dependent variable changes both its field name and the dependent variable name. If a new field name coincides with the name of another field of the same type, the fields share degrees of freedom and dependent variable names. A new field name must not coincide with the name of a field of another type or with a component name belonging to some other field. Component names must be unique within a model except when two fields share a common field name.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There are two *consistent stabilization methods*: **Streamline diffusion** and **Crosswind diffusion**. Usually, both checkboxes for these methods are selected by default and should remain selected for optimal performance. Consistent stabilization methods do not perturb the original transport equation. Streamline diffusion must be selected when using equal-order interpolation for pressure and velocity.

Select the **Use dynamic subgrid time scale** checkbox to estimate the influence of temporal variations in the velocity field, instead of using the inverse time step, in the consistent stabilization terms. This checkbox is selected by default

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps.

INCONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There is usually just one *inconsistent stabilization method* — **Isotropic diffusion**. This method is equivalent to adding a term to the diffusion coefficient in order to dampen the effect of oscillations by making the system somewhat less dominated by convection. If possible, minimize the use of the inconsistent stabilization method because by using it you no longer solve the original problem. By default, the **Isotropic diffusion** checkbox is not selected because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for underresolved problems.

If required, select the **Isotropic diffusion** checkbox and enter a **Tuning parameter** δ_{id} as a scalar positive value. The default value is 0.25 (a reasonable value to start with is roughly 0.5 divided by the element order). A higher value adds more isotropic diffusion.

- Numerical Stability — Stabilization Techniques for Fluid Flow

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

The **Use pseudo time stepping for stationary equation form** is per default set to **Automatic from physics**. This option can add pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. Pseudo time stepping is triggered when the Laminar Flow interface is selected in some multiphysics coupling features and for turbulent flows. Set **Automatic from physics** to **On** to apply pseudo time stepping also for laminar flows. Set it to **Off** to disable pseudo time stepping completely.

When **Use pseudo time stepping for stationary equation form** is set to **Automatic from physics** or **On**, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

The **Use Block Navier-Stokes preconditioner** checkbox under **Linear solver** is available when the **Compressibility** option is set to **Incompressible flow**. When this checkbox is selected, the default solver for time-dependent study steps will use the Block Navier–Stokes preconditioner in iterative solvers for the velocity and pressure. Using this preconditioner may result in shorter solution times for large time dependent problems with high Reynolds numbers.

- Pseudo Time Stepping for Laminar Flow Models
- Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow
- Theory for the Single-Phase Flow Interfaces
- Block Navier–Stokes in the *COMSOL Multiphysics Reference Manual.*

DISCRETIZATION

The default discretization for Laminar Flow is **P1+P1** elements — that is, piecewise linear interpolation for velocity and pressure. This is suitable for most flow problems.

Some higher-order interpolations are also available, and they can be cost-effective options to obtain high accuracy for flows with low Reynolds numbers.

The **P2+P2** and **P3+P3** options, the equal-order interpolation options, are the preferred higher-order options because they have higher numerical accuracy than the mixed-order options **P2+P1** and **P3+P2**. The equal-order interpolation options do, however, require streamline diffusion to be active.

Flow Past a Cylinder: Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow**

The Turbulent Flow, Algebraic yPlus Interface

The **Turbulent Flow, Algebraic yPlus (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for

incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Algebraic yPlus interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled wall distance. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation. When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

PHYSICAL MODEL

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** checkbox is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. Applying the **Fluid and Matrix Properties** on a subset of the domains enables studies of coupled porous-media flow and turbulent flow.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

Wall Treatment

Algebraic yPlus employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

The turbulence model parameters for the Algebraic yPlus model, κ_a and B_a, have been optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters. The turbulence model parameters can be tuned when the **Edit turbulence model parameters** checkbox is selected.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$
- **Pressure** p
- **Reciprocal wall distance** G
- **Wall distance in viscous units** yPlus (dimensionless)

The Algebraic yPlus interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual.*

The Turbulent Flow, L-VEL Interface

The **Turbulent Flow, L-VEL (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach number (typically less than 0.3).

The equations solved by the Turbulent Flow, L-VEL interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are included using an enhanced viscosity model based on the local wall distance, and the physics interface therefore includes a wall distance equation. When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**. Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

PHYSICAL MODEL

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** checkbox is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. Applying the **Fluid and Matrix Properties** on a subset of the domains enables studies of coupled porous-media flow and turbulent flow.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

Wall Treatment

L-VEL employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters, κ_l and E_l, have been optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters. The turbulence model parameters can be tuned when the **Edit turbulence model parameters** checkbox is selected.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Reciprocal wall distance** G
- **Tangential velocity in viscous units** uPlus (dimensionless)

The L-VEL interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Turbulent Flow, k-ε Interface

The **Turbulent Flow, k-ε (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, k-ε interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. The flow near walls is modeled using wall functions.

The Turbulent Flow, k-ε interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equation and the transport equations for k and ε, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties** and **Initial Values**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

Wall treatment for the k-ε model can only be set to **Wall functions**. More options becomes available by selecting another option under **Turbulence model**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1}, C_{e2}, C_{μ}, σ_{k}, σ_{e}, κ_{v}, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. The **Turbulence variables scale parameters** subsection is available when the **Turbulence model type** is set to **RANS-EVM** or **RANS-RSM**.

In addition to the settings described for the Laminar Flow interface, enter a value for U_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The U_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units, or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver.

- The Laminar Flow Interface
- Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Theory for the Turbulent Flow Interfaces

- *Airflow over an Ahmed Body*: Application Library path **CFD_Module/Verification_Examples/ahmed_body**
- *Pipe Erosion due to Contaminant Particles*: Application Library path **CFD_Module/Particle_Tracing/pipe_elbow_erosion**

Turbulent Flow over a Backward-Facing Step: Application Library path **Heat_Transfer_Module/Verification_Examples/turbulent_backstep**

The Turbulent Flow, Realizable k-ε Interface

The **Turbulent Flow, Realizable k-ε (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Realizable k-ε interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the realizable two-equation k-ε model. The flow near walls is modeled using wall functions.

The Turbulent Flow, Realizable k-ε interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equation and the transport equations for k and ε, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties** and **Initial Values**.

Except where included below, see The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_2, A_0, σ_k, σ_e, κ_v, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep

The Turbulent Flow, k-ω Interface

The **Turbulent Flow, k-ω (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, k-ω interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Wilcox revised two-equation k-ω model with realizability constraints. The k-ω model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall.

The Turbulent Flow, k-ω interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equation and the transport equations for the turbulent kinetic energy k and the specific dissipation ω, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall**, and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Wall Treatment

The k-ω model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. The most robust, but least accurate option is select the **Wall functions** option.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough. Observe that the **Low Re** formulation requires the wall distance to be solved for prior to the flow.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are α, σ_k^*, σ_w, β_0, β_0^*, κ_v, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Specific dissipation rate** om
- **Reciprocal wall distance** G

	Flow Through a Pipe Elbow: Application Library path **CFD_Module/Verification_Examples/pipe_elbow**

The Turbulent Flow, SST Interface

The **Turbulent Flow, SST (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, SST interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability constraints. The SST model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, SST interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Wall Treatment

The SST model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Include Transition Modeling

With this option enabled, the physics interface includes a local, correlation-based transition model. An additional transport equation for the intermittency is solved

together with the SST transport equations which are modified to include transition effects. This option requires **Low Re** wall treatment.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For this physics interface the turbulence model parameters are a_1, β_0^*, β_1, β_2, γ_1, γ_2, σ_{k1}, σ_{k2}, σ_{w1}, and σ_{w2}, and the transition model parameters (when **Include transition modeling** is enabled) are c_{e2}, c_{a2}, σ_γ, C_{TU1}, C_{TU2}, C_{TU3}, C_{PG1}, C_{PG2}, C_{PG3}, C_{PG1}^{lim}, C_{PG2}^{lim}, C_k, C_{SEP}, $Re_{\theta,c}^{lim}$.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Specific dissipation rate** om
- **Intermittency** gamma (when **Include transition modeling** is enabled)
- **Reciprocal wall distance** G

The **SST** interface requires a **Wall Distance Initialization** study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Turbulent Flow, Low Re k-ε Interface

The **Turbulent Flow, Low Re k-ε (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Low Re k-ε interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the AKN two-equation k-ε model with realizability constraints. The AKN model is a so-called low-Reynolds number model, which means that it can resolve the flow all the

way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, Low Re k-ε interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Wall Treatment

The AKN model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1}, C_{e2}, C_{μ}, σ_{k}, σ_{e}, and κ_{v}.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Turbulent kinetic energy** k

- **Turbulent dissipation rate** ep
- **Reciprocal wall distance** G

The Low Reynolds number k-ε interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- The Laminar Flow Interface
- Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Theory for the Turbulent Flow Interfaces

The Turbulent Flow, Spalart–Allmaras Interface

The **Turbulent Flow, Spalart–Allmaras (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Spalart–Allmaras interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Spalart–Allmaras one-equation model. The Spalart–Allmaras model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The Spalart–Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, Spalart–Allmaras interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equation and the transport equations for the undamped turbulent kinematic viscosity $\tilde{\nu}$, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall**, and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Wall Treatment

The Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{b1}, C_{b2}, C_{v1}, σ_{v}, C_{w2}, C_{w3}, κ_{v}, and C_{rot}.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Under the **Turbulence variables scale parameters** subsection, the default ν_{scale} is of the same order of magnitude as the kinematic viscosity of air at room temperature.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Reciprocal wall distance** G
- **Undamped turbulent kinematic viscosity** υ

The Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Turbulent Flow, v2-f Interface

The **Turbulent Flow, v2-f (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, v2-f interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the v2-f transport-equation model with realizability constraints. The v2-f model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The physics interface includes a wall distance equation.

The Turbulent Flow, v2-f interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-EVM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-RSM**, a turbulence model of RANS-RSM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Wall Treatment

The v2-f model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are $C_{\mu v2f}$, C_τ, C_η, C_L, C_1, C_2, $C_{\varepsilon 1 v2f}$, $C_{\varepsilon 2 v2f}$, A_1, σ_{kv2f}, $\sigma_{\varepsilon v2f}$, $\sigma_{\zeta v2f}$, κ_v, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep
- **Turbulent relative fluctuations** zeta
- **Elliptic blending function** alpha
- **Reciprocal wall distance** G

The v2-f interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- The Laminar Flow Interface
- Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Theory for the Turbulent Flow Interfaces

The Turbulent Flow, Wilcox R-ω Interface

The **Turbulent Flow, Wilcox R-ω (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible

flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Wilcox R-ω interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Wilcox R-ω seven-equation transport model. The Wilcox R-ω model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The physics interface includes a wall distance equation.

The Turbulent Flow, Wilcox R-ω interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-RSM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-EVM**, a turbulence model of RANS-EVM type can be selected under **Turbulence model**. Laminar or creeping flow can be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Wall Treatment

Low Re option, which enforces resolution all the way down to the wall, is used. This approach demands quite fine mesh near the wall.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are α, σ^*, σ_ω, β_{0W}, $\beta_0{}^*$, c_1^{PS} and c_2^{PS}.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field u** and its components
- **Pressure** p
- **Kinematic Reynolds stress, uu** uu

- **Kinematic Reynolds stress, vv** vv
- **Kinematic Reynolds stress, ww** ww
- **Kinematic Reynolds stress, uv** uv
- **Kinematic Reynolds stress, uw** uw
- **Kinematic Reynolds stress, vw** vw
- **Specific dissipation rate** om
- **Reciprocal wall distance** G

The Wilcox R-ω interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- The Laminar Flow Interface
- Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Theory for the Turbulent Flow Interfaces

The Turbulent Flow, SSG-LRR Interface

The **Turbulent Flow, SSG-LRR (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, SSG-LRR interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Speziale-Sarkar-Gatski/Launder-Reece-Rodi-ω (SSG-LRR) seven-equation transport model. The SSG-LRR model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The physics interface includes a wall distance equation.

The Turbulent Flow, SSG-LRR interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k-ε Interface for all the other settings.

TURBULENCE

A different turbulence model of RANS-RSM type can be selected under **Turbulence model**. Changing the **Turbulence model type** to **RANS-EVM**, a turbulence model of RANS-EVM type can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox, and for 2D components also the **Shallow Channel Approximation** checkbox.

Wall Treatment

Low Re option, which enforces resolution all the way down to the wall, is used. This approach demands quite fine mesh near the wall.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_μ, $\alpha_\omega^{(\omega)}$, $\alpha_\omega^{(\varepsilon)}$, $\beta_\omega^{(\omega)}$, $\beta_\omega^{(\varepsilon)}$, $\sigma_\omega^{(\omega)}$, $\sigma_\omega^{(\varepsilon)}$, $\sigma_d^{(\omega)}$, $\sigma_d^{(\varepsilon)}$, $c_1^{\mathrm{PS},(\omega)}$, $c_1^{\mathrm{PS},(\varepsilon)}$, $c_1^{\star,\,\mathrm{PS},(\omega)}$, $c_1^{\star,\,\mathrm{PS},(\varepsilon)}$, $c_2^{\mathrm{PS,LRR}}$, $c_2^{\mathrm{PS},(\omega)}$, $c_2^{\mathrm{PS},(\varepsilon)}$, c_3^{PS}, $c_3^{\star,\,\mathrm{PS},(\omega)}$, $c_3^{\star,\,\mathrm{PS},(\varepsilon)}$, $c_4^{\mathrm{PS},(\omega)}$, $c_4^{\mathrm{PS},(\varepsilon)}$, $c_5^{\mathrm{PS},(\omega)}$, $c_5^{\mathrm{PS},(\varepsilon)}$, $D^{(\omega)}$, and $D^{(\varepsilon)}$.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Kinematic Reynolds stress, uu** uu
- **Kinematic Reynolds stress, vv** vv
- **Kinematic Reynolds stress, ww** ww
- **Kinematic Reynolds stress, uv** uv
- **Kinematic Reynolds stress, uw** uw
- **Kinematic Reynolds stress, vw** vw
- **Specific dissipation rate** om
- **Reciprocal wall distance** G

The SSG-LRR interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- The Laminar Flow Interface
- Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Theory for the Turbulent Flow Interfaces

The LES RBVM Interface

The **LES RBVM (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers by resolving the larger three-dimensional unsteady eddies and modeling the effect of the smaller eddies using the residual-based variational multiscale (RBVM) method. The equations solved by the LES RBVM interface are the continuity equation for conservation of mass and the Navier–Stokes equation, augmented by additional stress terms, for conservation of momentum. Consistent modeling is used for the additional stresses. The interface is thus also applicable to laminar and transitional flows.

The LES RBVM interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes and continuity equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **LES model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS-EVM** or **RANS-RSM**, and a DES model can be selected by changing the **Turbulence model type** to **DES**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox and **Enable porous media domains** checkbox.

Wall Treatment

The LES RBVM model employs per default a **Low Re** wall treatment, which applies a Dirichlet condition for the velocity field.

Select the **Automatic** option in order to apply a tangential-stress condition based on a blending of asymptotic expressions in the viscous wall layer and the log layer. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Edit LES Model Parameters

Select this checkbox to edit the **L-VEL wall-treatment parameters**, κ_l and E_l, and the turbulence model parameter, C_μ, for the **Include synthetic turbulence** option in the **Velocity** inlet condition. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

The **Use dynamic subgrid time scale** checkbox is not selected by default.

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps. This checkbox is selected by default.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p

- The Laminar Flow Interface
- Theory for the Large Eddy Simulation Interfaces

The LES RBVMWV Interface

The **LES RBVMWV (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers by resolving the larger three-dimensional unsteady eddies and modeling the effect of the smaller eddies using the residual-based variational multiscale with viscosity (RBVMWV) method. The equations solved by the LES RBVMWV

interface are the continuity equation for conservation of mass and the Navier–Stokes equation, augmented by additional stress terms, for conservation of momentum. Similar modeling as for the LES RBVM model is applied but the effect of the Reynolds stress is enhanced by an additional residual-based diffusion term. Since the modeling is consistent, the interface is also applicable to laminar and transitional flows.

The LES RBVMWV interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes and continuity equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **LES model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS-EVM** or **RANS-RSM**, and a DES model can be selected by changing the **Turbulence model type** to **DES**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox and **Enable porous media domains** checkbox.

Wall Treatment

The LES RBVMWV model employs per default a **Low Re** wall treatment, which applies a Dirichlet condition for the velocity field.

Select the **Automatic** option in order to apply a tangential-stress condition based on a blending of asymptotic expressions in the viscous wall layer and the log layer. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Edit LES Model Parameters

Select this checkbox to edit the **L-VEL wall-treatment parameters**, κ_l and E_l, the additional diffusion parameter $\tilde{C}$, and the turbulence model parameter, C_μ, for the **Include synthetic turbulence** option in the **Velocity** inlet condition. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

The **Use dynamic subgrid time scale** checkbox is not selected by default.

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps. This checkbox is selected by default.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p

- The Laminar Flow Interface
- Theory for the Large Eddy Simulation Interfaces

The LES Smagorinsky Interface

The **LES Smagorinsky (spf)** interface ( ) is used for simulating single-phase flows at high Reynolds numbers by resolving the larger three-dimensional unsteady eddies and modeling the effect of the smaller eddies. The equations solved by the LES Smagorinsky interface are the continuity equation for conservation of mass and the Navier–Stokes equation, augmented by a turbulent viscosity term. The modeled term is inconsistent, which means that it does not vanish for a fully resolved flow.

The LES Smagorinsky interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes and continuity equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **LES model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS-EVM** or **RANS-RSM**, and

a DES model can be selected by changing the **Turbulence model type** to **DES**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox and **Enable porous media domains** checkbox.

Wall Treatment

The LES Smagorinsky model employs per default a **Low Re** wall treatment, which applies a Dirichlet condition for the velocity field.

Select the **Automatic** option in order to apply a tangential-stress condition based on a blending of asymptotic expressions in the viscous wall layer and the log layer. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Edit LES Model Parameters

Select this checkbox to edit the **L-VEL wall-treatment parameters**, κ_l and E_l, the Smagorinsky parameter C_s, and the turbulence model parameter, C_μ, for the **Include synthetic turbulence option** in the **Velocity** inlet condition. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

The **Use dynamic subgrid time scale** checkbox is not selected by default.

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps. This checkbox is selected by default.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p

- The Laminar Flow Interface
- Theory for the Large Eddy Simulation Interfaces

The DES RBVM, Spalart–Allmaras Interface

The **DES RBVM, Spalart–Allmaras (spf)** interface ( ) simulates turbulent single-phase flows by resolving the largest three-dimensional unsteady eddies and modeling the effect of the smaller eddies with the residual-based variational multiscale (RBVM) method in the bulk and with the Spalart–Allmaras model near walls. The equations solved by the DES RBVM, Spalart–Allmaras interface are the continuity equation for conservation of mass, the Navier–Stokes equation, augmented by additional stress terms, for conservation of momentum, and the Spalart–Allmaras equation for the undamped kinematic viscosity. Consistent modeling is used for the additional stresses.

The DES RBVM, Spalart–Allmaras interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes, continuity, and Spalart–Allmaras equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **LES model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS-EVM** or **RANS-RSM**, and a LES model can be selected by changing the **Turbulence model type** to **LES**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox and **Enable porous media domains** checkbox.

Wall Treatment

The DES RBVM, Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall-function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate that the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{μ}, for the **Include synthetic turbulence option** in the **Velocity** inlet condition and the Spalart–Allmaras parameters C_{b1}, C_{b2}, C_{v1}, $\sigma_{\tilde{\nu}}$, C_{w2}, C_{w3}, κ_{v}, B, and C_{DES}.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

The **Use dynamic subgrid time scale** checkbox is not selected by default.

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps. This checkbox is selected by default.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Reciprocal wall distance** G
- **Undamped turbulent kinematic viscosity** υ

The DES RBVM, Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Time Dependent study step.

- The Laminar Flow Interface
- Theory for the Detached Eddy Simulation Interfaces
- Theory for the Large Eddy Simulation Interfaces

The DES RBVMWV, Spalart–Allmaras Interface

The **DES RBVMWV, Spalart-Allmaras (spf)** interface ( ) simulates turbulent single-phase flows by resolving the largest three-dimensional unsteady eddies and modeling the effect of the smaller eddies with the residual-based variational multiscale method in the bulk and with the Spalart–Allmaras model near walls. The equations solved by

the DES RBVMWV, Spalart–Allmaras interface are the continuity equation for conservation of mass, the Navier–Stokes equation, augmented by additional stress terms, for conservation of momentum, and the Spalart–Allmaras equation for the undamped kinematic viscosity. Similar modeling as for the DES RBVM, Spalart–Allmaras model is applied but the effect of the Reynolds stress is enhanced by an additional residual-based diffusion term.

The DES RBVMWV, Spalart–Allmaras interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes, continuity, and Spalart–Allmaras equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **LES model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS-EVM** or **RANS-RSM**, and a LES model can be selected by changing the **Turbulence model type** to **LES**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox and **Enable porous media domains** checkbox.

Wall Treatment

The DES RBVMWV, Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall-function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate that the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_μ, for the **Include synthetic turbulence option** in the **Velocity** inlet condition, the additional diffusion parameter $\tilde{C}$, and the Spalart–Allmaras parameters C_{b1}, C_{b2}, C_{v1}, $\sigma_{\tilde{\nu}}$, C_{w2}, C_{w3}, κ_v, B, and C_{DES}.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

The **Use dynamic subgrid time scale** checkbox is not selected by default.

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps. This checkbox is selected by default.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Reciprocal wall distance** G
- **Undamped turbulent kinematic viscosity** υ

The DES RBVMWV, Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Time Dependent study step.

- The Laminar Flow Interface
- Theory for the Detached Eddy Simulation Interfaces
- Theory for the Large Eddy Simulation Interfaces

The DES Smagorinsky, Spalart–Allmaras Interface

The **DES Smagorinsky, Spalart–Allmaras (spf)** interface ( ) simulates turbulent single-phase flows by resolving the largest three-dimensional unsteady eddies and modeling the effect of the smaller eddies with the Smagorinsky model in the bulk and with the Spalart–Allmaras model near walls. The equations solved by the DES Smagorinsky, Spalart–Allmaras interface are the continuity equation for conservation of mass, the Navier–Stokes equation, augmented by a turbulent viscosity term, for conservation of momentum, and the Spalart–Allmaras equation for the undamped kinematic viscosity.

The DES Smagorinsky, Spalart–Allmaras interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes, continuity, and Spalart–Allmaras equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **LES model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS-EVM** or **RANS-RSM**, and a LES model can be selected by changing the **Turbulence model type** to **LES**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** checkbox and **Enable porous media domains** checkbox.

Wall Treatment

The DES Smagorinsky, Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall-function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate that the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{μ}, for the **Include synthetic turbulence option** in the **Velocity** inlet condition, the Smagorinsky parameter C_s, and the Spalart–Allmaras parameters C_{b1}, C_{b2}, C_{v1}, $\sigma_{\tilde{\nu}}$, C_{w2}, C_{w3}, κ_{ν}, B, and C_{DES}.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

The **Use dynamic subgrid time scale** checkbox is not selected by default.

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps. This checkbox is selected by default.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Reciprocal wall distance** G
- **Undamped turbulent kinematic viscosity** υ

The DES Smagorinsky, Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Time Dependent study step.

- The Laminar Flow Interface
- Theory for the Detached Eddy Simulation Interfaces
- Theory for the Large Eddy Simulation Interfaces

Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

The following nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- Boundary Stress
- Free Surface[2]
- Fan
- Flow Continuity
- Fluid-Fluid Interface[2]
- Fluid Properties
- Generate New Turbulence Model Interface
- Grille
- Gravity
- Initial Values
- Inlet
- Interior Fan
- Interior Wall
- Line Mass Source[1]
- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source[1]
- Porous Interface
- Pressure Point Constraint
- Screen
- Stationary Free Surface
- Symmetry
- Vacuum Pump
- Volume Force
- Wall

[1] A feature that may require an additional license

[2] See documentation for The Laminar Two-Phase Flow, Moving Mesh Interface

For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations solved by the physics interface, except for volume forces, which are added by the Volume Force feature. The node also provides an interface for defining the material properties of the fluid.

For the Turbulent Flow interfaces, the **Fluid Properties** node also adds the equations for the turbulence transport equations.

For the Viscoelastic Flow interface, the **Fluid Properties** node also adds the equations for the components of the elastic stress tensor.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the

value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p + p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

FLUID PROPERTIES

Density

The density can either be specified by a material, or by a **User defined** expression. The density in a material can depend on temperature and pressure, and these dependencies are automatically replaced by p_{ref} for weakly compressible flows and p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting at the physics interface level). If density variations with respect to pressure are to be included in the computations, **Compressibility** must be set to compressible. Any dependencies in the density on quantities other than temperature and pressure must be consistent with the **Compressibility** setting at the interface level.

Constitutive Relation

For laminar flow, the **Specify dynamic viscosity** (default) and **Inelastic non-Newtonian** options are available. Use the default option to either get the dynamic viscosity from a

material, or to add a user defined expression. The **Inelastic non-Newtonian** option includes several inelastic non-Newtonian models for the relationship between the shear stress and shear rate.

If the **Specify dynamic viscosity** option is selected, an inelastic non-Newtonian model can be selected by adding the corresponding **Material Properties** group as a subnode to a material node.

Dynamic Viscosity

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

Inelastic Non-Newtonian

Non-Newtonian fluids are encountered in everyday life and in a wide range of the industrial processes. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions. Such fluids have a nonlinear relationship between the shear stress and the share rate. The following inelastic non-Newtonian models are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou and Casson–Papanastasiou.

The following parameters are required for the **Power law**:

- **Fluid consistency coefficient** m
- **Flow behavior index** n
- **Lower shear rate limit** $\dot{\gamma}_{\mathrm{min}}$
- **Reference shear rate** $\dot{\gamma}_{\mathrm{ref}}$

For the **Carreau model**, the following parameters are required:

- **Zero shear rate viscosity** μ_0
- **Infinite shear rate viscosity** μ_{inf}
- **Relaxation time** λ
- **Power index** n

For the **Bingham–Papanastasiou model**, the following parameters are required:

- **Plastic viscosity** μ_{p}
- **Yield stress** τ_{y}
- **Model parameter** m_{p}

For the **Herschel–Bulkley–Papanastasiou model**, the following parameters are required:

- **Fluid consistency coefficient** m
- **Flow behavior index** n
- **Yield stress** τ_y
- **Reference shear rate** $\dot{\gamma}_{ref}$
- **Model parameter** m_p

For the **Casson–Papanastasiou model**, the following parameters are required:

- **Plastic viscosity** μ_p
- **Yield stress** τ_y
- **Model parameter** m_p

The default values for the parameters are listed in Table 3-2.

TABLE 3-2: DEFAULT VALUES FOR THE INELASTIC NON-NEWTONIAN MODELS.

NAME	UNIT	VARIABLE	DEFAULT VALUE
Fluid consistency coefficient	Pa·s	m	0.001
Flow behavior index / Power index	Dimensionless	n	1
Flow shear rate limit	s^{-1}	$\dot{\gamma}_{min}$	0.01
Reference shear rate	s^{-1}	$\dot{\gamma}_{ref}$	1
Zero shear rate viscosity	Pa·s	μ_0	0.001
Infinite shear rate viscosity	Pa·s	μ_{inf}	0
Relaxation time	s	λ	0
Plastic viscosity	Pa·s	μ_p	0.001
Yield stress	N/m^2	τ_y	0
Model parameter	s	m_p	10

- Non-Newtonian Flow

MIXING LENGTH LIMIT

For the Turbulent Flow, k-ε, Turbulent Flow, k-ω, and Rotating Machinery, Turbulent Flow k-ε interfaces, an upper limit on the mixing length is required.

When the **Mixing length limit** $l_{\text{mix,lim}}$ is set to **Automatic**, it is evaluated to the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually.

DISTANCE EQUATION

For the Turbulent Flow, Low Re k-ε; Turbulent Flow, k-ω with **Low Re** Wall Treatment; Turbulent flow, Algebraic yPlus; Turbulent Flow, L-VEL; Turbulent Flow, SST; Turbulent Flow, Spalart–Allmaras; Turbulent Flow, v2-f; Turbulent Flow, Wilcox, R-ω; Turbulent Flow, SSG-LRR interfaces Wall Distance interface is included.

When the **Reference length scale** l_{ref} is set to **Automatic**, it is evaluated to one tenth of the shortest side of the geometry bounding box. The solution to the wall distance equation is controlled by the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling because small objects would have too large an impact on the solution if the wall distance were measured exactly. The automatic value is usually a good choice but the value can become too high if the geometry consists of several slim entities. In such cases, it is recommended that the reference length scale is defined manually.

Volume Force

The **Volume Force** node specifies the volume force $\mathbf{F}$ on the right-hand side of the momentum equation.

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] + \mathbf{F}$$

If several volume-force nodes are added to the same domain, then the sum of all contributions are added to the momentum equation.

Initial Values

The initial values serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver in a stationary simulation. Note that for a transient compressible-flow simulation employing a material for which the density depends on the pressure (such as air), discontinuities in the initial values trigger pressure waves

even when the Mach number is small. The pressure waves must be resolved and this puts a restriction on the time step.

INITIAL VALUES

Initial values or expressions should be specified for the **Velocity field** $\mathbf{u}$ and the **Pressure** p.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p user input.

In the Turbulent Flow interfaces, initial values for the turbulence variables should also specified. Depending on the turbulent flow interface being used, additional initial values may be required for:

- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep
- **Reciprocal wall distance** G
- **Specific dissipation rate** om
- **Kinematic Reynolds stresses** uu, vv, ww, uv, uw, vw
- **Undamped turbulent kinematic viscosity** υ_0
- **Wall distance in viscous units** yPlus (dimensionless). Under normal circumstances the default value need not be changed.
- **Tangential velocity in viscous units** uPlus (dimensionless). Under normal circumstances the default value need not be changed.
- **Turbulent relative fluctuations** zeta
- **Elliptic blending function** alpha

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls. For turbulent flow, the description may involve wall functions and asymptotic expressions for certain turbulence variables.

BOUNDARY CONDITION

Select a **Boundary condition** for the wall.

- No Slip
- Slip
- Slip Velocity
- Leaking Wall
- Navier Slip

No Slip

No slip is the default boundary condition to model solid walls. A no-slip wall is a wall where the fluid velocity relative to the wall velocity is zero. For a stationary wall that means that $\mathbf{u} = 0$.

For turbulent flows, the no-slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall treatment** is set to **Wall functions**, the **Apply wall roughness** option becomes available. When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. Select **Generic roughness** in order to specify more general roughness types.

- For **Sand roughness** an **Equivalent sand roughness height** k_{seq} should be specified.
- For **Generic roughness** a **Roughness height** k_{s} and a dimensionless **Roughness parameter** C_{s} should be specified.

The option for **Porous treatment of no slip condition** is available when **Enable porous media domains** is activated in the **Physical Model** section in the settings for the main physics interface node. It specifies how **Wall** boundaries and **Interior Wall** boundaries adjacent to porous domains are treated. When **Standard no slip formulation** is chosen, a common no slip condition is applied on all solid walls. When the default **Porous slip** is chosen, a blending analytic expression is instead applied on the corresponding wall boundaries adjacent to the porous medium domain. It results in a no slip condition in case the porous length scale is fully resolved by the mesh and a slip condition in the opposite limit when the mesh is much coarser than the porous scale. A smooth transition between these limits is ensured. Note that the interpretation and usage of nonzero slip at the wall is the same as in the **Navier slip** boundary condition. By default, **Velocity formulation** is on and the treatment is based on an approximate reconstruction of the far-field pressure gradient using the slip velocity at the wall. If the **Pressure-gradient formulation** is chosen, the local pressure gradient at the wall is employed.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u}\cdot\mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Slip Velocity

In the microscale range, the flow condition at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a **Slip velocity** at the boundary. Two phenomena account for this velocity: noncontinuum effects and the flow induced by a thermal gradient along the boundary.

When the **Use viscous slip** checkbox is selected, the default **Slip length** L_s is **User defined**. Another value or expression may be entered if the default value is not applicable. For **Maxwell's model** values or expressions for the **Tangential momentum accommodation coefficient** a_v and the **Mean free path** λ should be specified. Tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

When the **Use thermal creep** checkbox is selected, a thermal creep contribution with **Thermal slip coefficient** σ_T is activated. Thermal slip coefficients are typically between 0.3 and 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

Slip velocity is available when **Turbulence Model** in the **Turbulence** section of the interface is set to **None**.

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_l$ through a perforated wall. The components of the **Fluid velocity** $\mathbf{u}_l$ on the leaking wall should be specified.

Leaking Wall is available when **Turbulence Model** in the **Turbulence** section of the interface is set to **None**.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$, and adds a tangential stress

$$\mathbf{K}_{\text{nt}} = -\frac{\mu}{\beta}\mathbf{u}_{\text{slip}}$$

where $\mathbf{K}_{nt} = \mathbf{K}_n - (\mathbf{K}_n \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$, $\mathbf{K}_n = \mathbf{K}\mathbf{n}_{wall}$, and $\mathbf{K}$ is the viscous stress tensor. β is a slip length, and $\mathbf{u}_{slip} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ is the velocity tangential to the wall.

The **Slip length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side and f_h is a user input. Select **User defined** from the **Slip length** selection list in order to manually prescribe β (SI unit: m).

In cases where the wall movement is nonzero, select the **Account for the translational wall velocity of the wall in the friction force** checkbox to use $\mathbf{u} - \mathbf{u}_{bnd} - ((\mathbf{u} - \mathbf{u}_{bnd}) \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ instead of $\mathbf{u}_{slip}$ in the friction force.

The Navier slip option is not available when selecting a turbulence model.

For the Viscoelastic Flow interface, $\mathbf{K}_n$ is the sum of the viscous and the elastic contributions.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{tr}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{tr} = \mathbf{0}$. If the frame moves, $\mathbf{u}_{tr}$ becomes equal to the frame movement. $\mathbf{u}_{tr}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Zero (Fixed wall)** from **Translational velocity** selection list to prescribe $\mathbf{u}_{tr} = \mathbf{0}$.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u}_{tr}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh node needs to be added from Definitions to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt with the surface sliding in a tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall** $\mathbf{u}_w$ should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL

Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.

- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.
- For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the **Velocity of moving wall**, **φ-component** v_w can also be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options** in the **Show More Options** dialog. The **Constraints** settings can be set to **Automatic**, **Pointwise constraints**, **Nitsche constraints**, or **Weak constraints**. **Mixed constraints** can be selected when imposing a no slip condition exactly.

Depending on the constraint method selected, the following settings are available:

- **Apply reaction terms on** can be set to **Individual dependent variables** (default) or **All physics (symmetric)**. This setting is not available when **Nitsche constraints** or, for the **Slip Flow (slpf)** interface, **Weak constraints** is selected.
- Select **Elemental** (default) or **Nodal** under **Constraint method**. This setting is not available for **Nitsche constraints** or **Weak constraints**.

- Theory for the Wall Boundary Condition
- The Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Inlet

This condition should be used on boundaries for which there is a net flow into the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Outlet conditions when specifying an Inlet condition. For example, if the pressure is specified at the outlet, the velocity may be specified at the inlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties.

BOUNDARY CONDITION

The available **Boundary condition** options for an inlet are **Velocity, Fully developed flow**, **Mass flow**, and **Pressure**. After selecting a **Boundary Condition** from the list, a section with the same or a similar name displays underneath. For example, if **Velocity** is selected, a **Velocity** section, where further settings are defined, is displayed.

VELOCITY

The **Normal inflow velocity** is specified as $\mathbf{u} = -\mathbf{n}U_0$, where $\mathbf{n}$ is the boundary normal pointing out of the domain and U_0 is the normal inflow speed.

The **Velocity field** option sets the velocity vector to $\mathbf{u} = \mathbf{u}_0$. The components of the inlet velocity vector $\mathbf{u}_0$ should be defined for this choice.

The **Include synthetic turbulence** option is available when the **Turbulence Model Type** is set to **Large Eddy Simulation** or **Detached Eddy Simulation**. It is disabled by default. When it is enabled, the **Normal inflow velocity** is specified as $\mathbf{u} = -\mathbf{n}U_0 + \mathbf{u}'_{\text{in,t}}$, and the **Velocity field** option sets the velocity vector to $\mathbf{u} = \mathbf{u}_0 + \mathbf{u}'_{\text{in,t}}$, where $\mathbf{u}'_{\text{in,t}}$ is the fluctuating inlet velocity at time t. The section titled **Turbulence Conditions** controls the parameters that determine the fluctuating velocity.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure.

- For incompressible flow, the **Pressure** list has two options, **Static** and **Total**. For weakly compressible and compressible flow, the static pressure should be specified in the text field.
  - If **Pressure** is **Static**, and the reference pressure p_{ref}, defined at the physics interface level, is equal to 0, the value of the pressure p_0, at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.
  - If **Pressure** is **Total**, the **Average** checkbox is available and cleared by default to prescribe the total pressure pointwise. If it is selected, the averaged total pressure is imposed in the weak forms instead.

  When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is

available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The **Suppress backflow** option adjusts the inlet pressure locally in order to reduce the amount of fluid exiting the domain through the boundary. If you clear the suppress backflow option, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.
- **Flow direction** controls in which direction the fluid enters the domain.
  - For **Normal flow**, it prescribes zero tangential velocity component.
  - For **User defined**, an **Inflow velocity direction** $\mathbf{d_u}$ (dimensionless) should be specified. The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.

MASS FLOW

The mass flow at an inlet can be specified by the **Mass flow rate**, the **Pointwise mass flux**, the **Standard flow rate**, or the **Standard flow rate (SCCM)**.

The **Apply condition on each disjoint selection separately** checkbox is selected per default. When this setting is selected, the mass flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

Mass Flow Rate

The **Mass flow rate** option sets the integrated mass flow over the boundary selection, the **Normal mass flow rate** to a specific value, m. The mass flow is assumed to be parallel to the boundary normal, and the tangential flow velocity is set to zero.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Pointwise Mass Flux

The **Pointwise mass flux** sets the mass flow parallel to the boundary normal. The tangential flow velocity is set to zero. The mass flux is a model input, which means that COMSOL Multiphysics can take its value from another physics interface when

available. When **User defined** is selected a value or function M_f should be specified for the **Mass flux**.

Standard Flow Rate

The **Standard flow rate** Q_{sv} sets a standard volumetric flow rate, according to the SEMI standard E12-0303. The mass flow rate is specified as the volumetric flow rate of a gas at standard density — the **Mean molar mass** M_n divided by a **Standard molar volume** V_{m} (that is, the volume of one mole of a perfect gas at standard pressure and standard temperature). The flow occurs across the whole boundary in the direction of the boundary normal and is computed by a surface (3D) or line (2D) integral. The tangential flow velocity is set to zero.

The standard density can be defined directly, or by specifying a standard pressure and temperature, in which case the ideal gas law is assumed. The options in the **Standard flow rate defined by** list are:

- **Standard density**, for which the **Standard molar volume** V_{m} should be specified.
- **Standard pressure and temperature**, for which the **Standard pressure** P_{st} and the **Standard temperature** T_{st} should be defined.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Standard Flow Rate (SCCM)

The **Standard flow rate (SCCM)** boundary condition is equivalent to the **Standard flow rate** boundary condition, except that the flow rate is entered directly in SCCMs (standard cubic centimeters per minute) without the requirement to specify units. Here, the dimensionless **Number of SCCM units** Q_{sccm} should be specified.

FULLY DEVELOPED FLOW

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow toward the solution for a fully developed channel flow. The channel can be thought of as a virtual extrusion of the inlet cross section. The inlet boundary must hence be flat in order for the fully developed flow condition to work properly. In 2D axisymmetric models, the inlet normal must be parallel to the symmetry axis.

Select an option to control the flow rate at the inlet:

- **Average velocity**, U_{av}.

- **Flow rate**, V_0. Two-dimensional models also require an **Entrance thickness**, D_z, which is the out-of-plane thickness of the extruded entrance channel.
- **Average pressure**, P_{av}. Note that P_{av} is the average pressure on the inflow boundary.

The **Apply condition on each disjoint selection separately** checkbox is selected per default. When this setting is selected, the fully developed flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the inlet boundary. The exception is gravity when the **Include gravity** setting is selected in the physics interface settings. Unless **Use reduced pressure** is also selected, an option to **Compensate for hydrostatic pressure** or **Compensate for hydrostatic pressure approximation** becomes available. It is selected per default and should only be deselected if the inlet normal is aligned with the gravity force and you want to specify an average pressure that includes the hydrostatic pressure.

Fully developed inflow can be used in conjunction with the turbulence models, except for RANS-RSM type of turbulence models. No additional inputs are required for the turbulence variables. They are instead solved for on the inlet boundary to be consistent with the fully developed flow profile.

For the Viscoelastic Flow interface, the fully developed inflow can be used in conjunction with the viscoelastic constitutive model. No additional inputs are required for the elastic stress tensor components. They are instead solved for on the inlet boundary to be consistent with the fully developed flow profile.

TURBULENCE CONDITIONS

No additional inlet conditions are required for the algebraic turbulence models: Algebraic yPlus and L-VEL.

For the **Turbulent Flow, Spalart–Allmaras** interface, a value or expression for the **Undamped turbulent kinematic viscosity** υ_0 should be specified.

For transport-equation turbulence models, apart from the Spalart–Allmaras turbulence model, the following settings are available under the **Specify turbulence length scale and intensity** option (see Table 3-3 for the default values):

- **Turbulent intensity** I_{T}

- **Turbulence length scale** L_T
- **Reference velocity scale** U_{ref}

When **Include transition modeling** is selected in the SST turbulence model, the intermittency, γ, is set to 1. For the v2-f turbulence model and any turbulence model of RANS-RSM type, the additional choice between **Isotropic turbulence** and **Specify turbulence anisotropy** appears. With **Specify turbulence anisotropy**, a value for the turbulent relative fluctuations at the inlet, ζ_0, may be specified for v2-f turbulence model, while a RANS-RSM allows to specify a_0, the turbulence anisotropy tensor. When **Specify turbulence variables** is selected, values or expressions for the dependent turbulence variables should be defined. Availability is based on the physics interface and the boundary condition chosen.

- **Turbulent kinetic energy** k_0
- **Turbulent dissipation rate** ε_0
- **Specific dissipation rate** ω_0
- **Kinematic Reynolds stress tensor** R_0
- **Turbulent relative fluctuations** ζ_0
- **Elliptic blending function** α_0
- **Intermittency** γ_0

TABLE 3-3: DEFAULT VALUES FOR THE TURBULENT INTERFACES.

NAME AND UNIT	VARIABLE	INLET	OPEN BOUNDARY	BOUNDARY STRESS
Turbulent intensity (dimensionless)	I_T	Medium	0.005	0.01
Turbulence length scale (m)	L_T	Geometry based	0.1	0.1
Reference velocity scale (m/s)	U_{ref}	1	1	1
Turbulent kinetic energy (m^2/s^2)	k_0	0.005	$2.5 \cdot 10^{-3}$	$1 \cdot 10^{-2}$
Turbulent dissipation rate (m^2/s^3)	ε_0	0.005	$1.1 \cdot 10^{-4}$	$1 \cdot 10^{-3}$
Specific dissipation rate (1/s)	ω_0	20	0.5	0.5
Undamped turbulent kinematic viscosity (m^2/s)	υ_0	`3*spf.nu`		
Intermittency (dimensionless)	γ_0	1		

For the Large Eddy Simulation and Detached Eddy Simulation interfaces, when the **Include synthetic turbulence** option is selected, the **Number of Fourier modes** is specified as an integer value greater than or equal to 2 in order to control the number of Fourier modes used in the generation of the fluctuating inlet velocity.

When the **Use random seed** checkbox is enabled, one can specify the value of a **Random seed**, r, which is used in randomly generating various angles that determine the orientation of the fluctuating velocity.

For a detailed formulation of the generation of inlet turbulent fluctuations, see Synthetic Turbulence Inlet Condition section.

About the Turbulent Intensity and Turbulence Length Scale Parameters

The **Turbulent intensity** I_T and **Turbulence length scale** L_T values are related to the turbulence variables via the following equations, Equation 3-2 for the Inlet and Equation 3-3 for the Open Boundary:

$$\text{Inlet } k = \frac{3}{2}(|\mathbf{U}|I_T)^2, \qquad \varepsilon = C_\mu^{3/4}\frac{k^{3/2}}{L_T} \tag{3-2}$$

$$\text{Open Boundary } k = \frac{3}{2}(I_T U_{ref})^2, \qquad \varepsilon = \frac{C_\mu^{3/4}}{L_T}\left(\frac{3(I_T U_{ref})^2}{2}\right)^{\frac{3}{2}} \tag{3-3}$$

For the Open Boundary and Boundary Stress options, and with any Turbulent Flow interface, inlet conditions for the turbulence variables also need to be specified. These conditions are used on the parts of the boundary where $\mathbf{u} \cdot \mathbf{n} < 0$, that is, where flow enters the computational domain.

For the **k-ω** and **SST** turbulence models the **Turbulent intensity** I_T and **Turbulence length scale** L_T values are related to the turbulence variables via the following equations, Equation 3-4 for the Inlet and Equation 3-5 for the Open Boundary:

$$\text{Inlet } k = \frac{3}{2}(|\mathbf{U}|I_T)^2, \qquad \omega = \frac{\sqrt{k}}{(\beta_0^*)^{1/4}L_T} \tag{3-4}$$

$$\text{Open Boundary } k = \frac{3}{2}(I_T U_{ref})^2, \qquad \omega = \frac{1}{(\beta_0^*)^{1/4}L_T}\sqrt{\left(\frac{3(I_T U_{ref})^2}{2}\right)} \tag{3-5}$$

For Wilcox **R-ω** turbulence model the **Turbulent intensity** I_T and **Turbulence length scale** L_T values are related to the turbulence variables via the following equations, Equation 3-6 for the Inlet and Equation 3-7 for the Open Boundary:

$$\text{Inlet } R_{ij} = (|\mathbf{U}|I_T)^2\delta_{ij}, \qquad \omega = \frac{\sqrt{k}}{(\beta_0^*)^{1/4}L_T} \tag{3-6}$$

$$\text{Open Boundary } R_{ij} = (I_T U_{\text{ref}})^2\delta_{ij}, \qquad \omega = \frac{1}{(\beta_0^*)^{1/4}L_T}\sqrt{\left(\frac{3(I_T U_{\text{ref}})^2}{2}\right)} \tag{3-7}$$

For SSG-LRR turbulence model, Equation 3-6 for the Inlet and Equation 3-7 for the Open Boundary are valid except $\beta_0^* \rightarrow C_\mu$.

For the inlet, I_T and L_T can be chosen in the lists. There are:

- Four options for I_T: **Low** (0.01), **Medium** (0.05), **High** (0.1), and **User defined**.
- Two options for L_T: **Geometry based**, and **User defined**. In the **Geometry based** option, it is automatically computed based on 7% of the hydraulic diameter.

VISCOELASTIC STRESS

For the Viscoelastic Flow interface, the inlet conditions for the elastic stress components are required. Note, that if several branches are specified in the **Fluid Property** node, the initial values entered above are applied to all branches.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

- Prescribing Inlet and Outlet Conditions
- Normal Stress Boundary Condition

For recommendations of physically sound values for the **Turbulent intensity** I_T and **Turbulence length scale** L_T, see Inlet Values for the Turbulence Length Scale and Turbulent Intensity.

Fully Developed Flow (Inlet)

Stationary Incompressible Flow over a Backstep (inlet): Application Library path **CFD_Module/Single-Phase_Flow/backstep**

Outlet

This condition should be used on boundaries for which there is a net outflow from the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Inlet conditions when specifying an Outlet condition. For example, if the velocity is specified at the inlet, the pressure may be specified at the outlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties. Selecting appropriate outlet conditions for the Navier–Stokes equations is a nontrivial task. Generally, if there is something interesting happening at an outflow boundary, the computational domain should be extended to include this phenomenon.

BOUNDARY CONDITION

The available **Boundary condition** options for an outlet are **Pressure, Velocity, Fully developed flow**, and **Mass flow**.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure. The tangential stress component is set to zero.

- For incompressible flow, the **Pressure** list has two options, **Static** and **Total**. For weakly compressible and compressible flow, the static pressure should be specified in the text field.
  - If **Pressure** is **Static**, and the reference pressure p_{ref}, defined at the physics interface level, is equal to 0, the value of the pressure p_0, at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.
  - If **Pressure** is **Total**, the **Average** checkbox is available and selected by default to prescribed the averaged total pressure in the weak forms. If it is cleared, the total pressure is imposed pointwise.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and

selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The **Normal flow** option changes the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The **Suppress backflow** checkbox is selected by default. This option adjusts the outlet pressure in order to reduce the amount of fluid entering the domain through the boundary.

VELOCITY

See the **Inlet** node Velocity section for the settings.

FULLY DEVELOPED FLOW

This boundary condition is applicable when the flow exits the domain into a long pipe or channel, at the end of which a flow profile is fully developed.

The channel can be thought of as a virtual extrusion of the outlet cross section. The outlet boundary must hence be flat in order for the fully developed flow condition to work properly. In 2D axisymmetric models, the outlet normal must be parallel to the symmetry axis.

Select an option to control the flow rate at the outlet:

- **Average velocity**, U_{av}.
- **Flow rate**, V_0. Two-dimensional models also require an **Entrance thickness**, D_z, which is the out-of-plane thickness of the extruded entrance channel.
- **Average pressure**, P_{av}. Observe that P_{av} is the average pressure on the outflow.

The **Apply condition on each disjoint selection separately** checkbox is selected per default. When this setting is selected, the fully developed flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the outlet boundary. The exception is gravity when the **Include gravity** setting is selected in the physics interface settings. Unless **Use reduced pressure** is also selected, an option to **Compensate for hydrostatic pressure** or **Compensate for hydrostatic pressure approximation** becomes available. It is selected per

default and should only be deselected if the outlet normal is aligned with the gravity force and you want to specify an average pressure that includes the hydrostatic pressure.

Fully developed outflow can be used in conjunction with the turbulence models, except for RANS-RSM type. No additional inputs are required for the turbulence variables. They are instead solved for on the outlet boundary to be consistent with the fully developed flow profile.

For the Viscoelastic Flow interface, the fully developed outflow can be used in conjunction with the viscoelastic constitutive model. No additional inputs are required for the elastic stress tensor components. They are instead solved for on the outlet boundary to be consistent with the fully developed flow profile.

MASS FLOW

See the **Inlet** node Mass Flow section for the settings.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

	Prescribing Inlet and Outlet Conditions

	Fully Developed Flow (Outlet)

Symmetry

This node provides a boundary condition for symmetry boundaries. It should only be used when the geometry and expected solution have mirror symmetry. By using symmetries in a model its size can be reduced by one-half or more, making this an efficient tool for solving large problems.

The **Symmetry** boundary condition prescribes no penetration and vanishing shear stresses. The boundary condition is a combination of a Dirichlet condition and a Neumann condition:

$$\mathbf{u}\cdot\mathbf{n} = 0, \qquad \left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{0}$$

$$\mathbf{u}\cdot\mathbf{n} = 0, \qquad (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}))\mathbf{n} = \mathbf{0}$$

for the compressible and incompressible formulations. The Dirichlet condition takes precedence over the Neumann condition, and the above equations are equivalent to the following equation for both the compressible and incompressible formulations:

$$\mathbf{u}\cdot\mathbf{n} = 0, \qquad \mathbf{K} - (\mathbf{K}\cdot\mathbf{n})\mathbf{n} = \mathbf{0}$$
$$\mathbf{K} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}})\mathbf{n}$$

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at $r = 0$. The software automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the z direction and adds an **Axial Symmetry** node that implements these conditions on the axial symmetry boundaries only.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

Open Boundary

The **Open Boundary** condition describes boundaries in contact with a large volume of fluid. Fluid can both enter and leave the domain on boundaries with this type of condition.

BOUNDARY CONDITIONS

The **Boundary condition** options for open boundaries are **Normal stress** and **No viscous stress**.

Normal Stress

The **Normal stress** f_0 condition implicitly imposes $p \approx \mathrm{f}_0$.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 user input.

No Viscous Stress

The **No Viscous Stress** condition specifies vanishing viscous stress on the boundary. This condition does not provide sufficient information to fully specify the flow at the open boundary and must at least be combined with pressure constraints at adjacent points.

The **No viscous stress** condition prescribes:

$$\left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{0}$$

$$\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} = \mathbf{0}$$

for the compressible and the incompressible formulations. This condition can be useful in some situations because it does not impose any constraint on the pressure. A typical example is a model with volume forces that give rise to pressure gradients that are hard to prescribe in advance. To make the model numerically stable, this boundary condition should be combined with a point constraint on the pressure.

TURBULENCE CONDITIONS

See Turbulence conditions.

VISCOELASTIC STRESS

For Viscoelastic Flow interface, **Viscoelastic Stress** section is available. See Viscoelastic Stress.

Boundary Stress

The **Boundary Stress** node adds a boundary condition that represents a general class of conditions also known as traction boundary conditions.

BOUNDARY CONDITION

The **Boundary condition** options for the boundary stress are **General stress**, **Normal stress**, and **Normal stress, normal flow**.

General Stress

When **General stress** is selected, the components for the **Stress** $\mathbf{F}$ should be specified. The total stress on the boundary is set equal to the given stress $\mathbf{F}$:

$$\left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{F}$$

$$(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = \mathbf{F}$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n} - \mathbf{n}\cdot\mathbf{F} \tag{3-8}$$

If $\partial u_n/\partial n$ is small, Equation 3-8 states that $p \approx -\mathbf{n}\cdot\mathbf{F}$.

Normal Stress

Normal Stress is described for the Open Boundary node.

Normal Stress, Normal Flow

For **Normal stress, normal flow**, the magnitude of the **Normal stress** f_0 should be specified. The tangential velocity is set to zero on the boundary:

$$\mathbf{n}^T\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -f_0, \qquad \mathbf{t}\cdot\mathbf{u} = 0$$

$$\mathbf{n}^T(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -f_0, \qquad \mathbf{t}\cdot\mathbf{u} = 0$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n} + f_0 \tag{3-9}$$

If $\partial u_n/\partial n$ is small, Equation 3-9 states that $p \approx f_0$.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 or $p_{\text{hydro}}\mathbf{n}$ is added to $\mathbf{F}$ depending on the selected option.

Turbulent Boundary Type

The **Turbulent boundary type** options for this boundary condition are **Open boundary**, **Inlet**, and **Outlet**.

- For **Open boundary** parts of the boundary are expected to be outlets and other parts are expected to be inlets.
- The **Inlet** option should be selected when the whole boundary is expected to be an inlet.
- The **Outlet** option should be used when the whole boundary is expected to be an outflow boundary. In this case, homogeneous Neumann conditions are applied for the turbulence variables, that is, for k and ε

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla \varepsilon \cdot \mathbf{n} = 0$$

and additionally for the v2-f model

$$\nabla \alpha \cdot \mathbf{n} = 0 \qquad \nabla \zeta \cdot \mathbf{n} = 0$$

for k and ω

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla \omega \cdot \mathbf{n} = 0$$

for RANS-RSM type of turbulence models

$$\nabla R_{ij} \cdot \mathbf{n} = 0 \qquad \nabla \omega \cdot \mathbf{n} = 0$$

for the Spalart–Allmaras model

$$\nabla \tilde{\nu} \cdot \mathbf{n} = 0$$

and for the SST model when **Include transition modeling** is selected

$$\nabla \gamma \cdot \mathbf{n} = 0$$

TURBULENCE CONDITIONS

See Turbulence conditions.

VISCOELASTIC STRESS

For Viscoelastic Flow interface, **Viscoelastic Stress** section is available. See Viscoelastic Stress.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

If Normal Stress, Normal Flow is selected as the **Boundary condition**, then to **Apply reaction terms on** all dependent variables, the **All physics (symmetric)** option should be selected. Alternatively, the **Individual dependent variables** could be selected to restrict the reaction terms as needed.

Screen

The **Screen** condition models interior wire gauzes, grilles, or perforated plates as thin permeable barriers. Common correlations are included for resistance and refraction coefficients. The Screen boundary condition can only be applied on interior boundaries.

SCREEN TYPE

The available options for the **Screen type** are **Wire gauze**, **Square mesh**, **Perforated plate**, and **User defined**. The settings are defined by the equations shown based on the selection (excluding User defined) which in turn adjusts what is available in the **Parameters** section.

PARAMETERS

If **Wire gauze**, **Square mesh**, or **Perforated plate** is selected as the **Screen type**, values or expressions for the **Solidity** σ_s (ratio of blocked area to total area of the screen) should be specified.

- For **Wire gauze** a value or expression for the **Wire diameter** d should also be specified.
- The **User defined** options requires the dimensionless **Resistance coefficient** K.
- For all screen types, the **Refraction** defaults to **Wire gauze**. With the **User defined** option, a different **Refraction coefficient** η (dimensionless) can be specified.

- Screen Boundary Condition
- Theory for the Nonisothermal Screen Boundary Condition

Vacuum Pump

The **Vacuum Pump** node models the effective outlet volume flow rate created by a vacuum pump device that is attached to an outlet.

PARAMETERS

The **Flow condition** option defines a lumped curve — **Vacuum pump performance curve, linear**; **Vacuum pump performance curve, data**; or **Vacuum pump performance curve, user defined**.

Vacuum Pump Performance Curve, Linear

For the **Vacuum pump performance curve, linear** option, values or expressions should be specified for the **Ultimate pressure** p_{ult} and the **Pumping rate at ambient pressure** $V_{0,\mathrm{amb}}$.

The vacuum pump performance curve value is equal to 0 when the suction pressure is smaller than p_{ult}, and equal to $V_{0,\mathrm{amb}}$ when the suction pressure is larger than the ambient pressure.

Vacuum Pump Performance Curve, Data

The **Vacuum pump performance curve, data** option can be used to enter or load data under the **Vacuum Pump Performance Curve Data** section below. The interpolation between points given in the **Vacuum Pump Performance Curve Data** table is defined using the **Interpolation function type** list in the **Vacuum Pump Performance Curve Interpolation** section.

Vacuum Pump Performance Curve, User Defined

The **Vacuum pump performance curve, user defined** option can be used to enter a different value or expression. The suction pressure on the selection where this boundary condition is applied is defined by *phys_id*`.`*item.id*`.pAverage` where *phys_id* is the name of the physics interface and *item.id* is the name of the feature (for example, *phys_id* is `spf` and *item.id* is `pmp1` by default for the first instance of the **Vacuum pump** boundary condition in the single-phase flow physics interface). In order to avoid unexpected behavior, the function used for the vacuum pump performance curve is the maximum of the user-defined function and 0.

VACUUM PUMP PERFORMANCE CURVE DATA

This section displays when **Vacuum pump performance curve, data** is selected as the **Flow condition**. In the table, values or expressions for the **Suction pressure** and **Pumping rate** should be specified. Alternatively, a text file can be imported by clicking the **Load from file** button ( ) under the table.

UNITS

This section is available when **Vacuum pump performance curve, data** is selected as the **Flow condition**. Units can be specified here for the **Suction pressure** and **Pumping rate**.

VACUUM PUMP PERFORMANCE CURVE INTERPOLATION

This section is available when **Vacuum pump performance curve, data** is selected as the **Flow condition**. The available options for the **Interpolation function type** are **Linear**, **Piecewise cubic**, and **Cubic spline**.

The extrapolation method always returns a constant value. In order to avoid problems with undefined data, the function used for the boundary condition is the maximum of the interpolated function and 0.

Vacuum Pump Boundary Condition

The **Vacuum Pump** feature computes the flux across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several pumps on boundaries that are not connected, it is good practice to use different Vacuum Pump features with connected boundaries.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group (the **Destination Selection** section is optional). Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

No input is required when **Compressible flow (Ma<0.3)** is selected for **Compressibility** under the **Physical Model** section for the physics interface. Typically when a periodic boundary condition is used with a compressible flow, the pressure is the same at both boundaries and the flow is driven by a volume force.

BOUNDARY SELECTION

The software usually automatically identifies the boundaries as either source boundaries or destination boundaries, as indicated in the selection list. This works fine for cases like opposing parallel boundaries. In other cases, right-click **Periodic Flow Condition** and select **Manual Destination Selection** to control the destination. By default it contains the selection that COMSOL Multiphysics identifies.

DESTINATION SELECTION

This section is available for specifying the destination boundaries, if needed, when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Flow Condition** node. You can only select destination boundaries from the union of all source and destination boundaries.

FLOW CONDITION

This section is available when **Incompressible flow** is selected for **Compressibility** under the **Physical Model** section for the physics interface.

The **Flow Condition** at the boundary is specified through a value or expression for either the **Pressure difference**, $p_{\mathrm{src}} - p_{\mathrm{dst}}$, or the **Mass flow**, $\dot{m}$. The mass flow option ensures a pressure difference is achieved across the source and destination boundaries. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual.*

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics**

Options is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping Between Source and Destination** section, see Mapping Between Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Fan

The **Fan** condition is used to define the flow direction (inlet or outlet) and the fan parameters on exterior boundaries. The Interior Fan condition is available on interior boundaries.

FLOW DIRECTION

The **Flow direction** can be set to **Inlet** or **Outlet**. When a boundary has been selected, an arrow displays in the **Graphics** window to indicate the selected flow direction. The arrow can be updated if the selection changes by clicking any node in the **Model Builder** and then clicking the **Fan** node again to update the **Graphics** window.

The **Inlet Flow direction** controls in which direction the fluid enters the domain.

- For **Normal flow** it sets the tangential velocity component to zero.
- For **User defined** an **Inflow velocity direction** $\mathbf{d_u}$ (dimensionless) should be specified. The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.
- For **Swirl flow** (which is available for 3D or 2D axisymmetric when the **Swirl flow** checkbox in the **Physical Model** section is selected) it specifies a swirl flow on the downstream side of the fan based on the **Rotation axis base point** $\mathbf{r}_{\mathrm{bp}}$, **Revolutions per time** f, **Rotational direction**, and **Swirl ratio** c_{sf}.

PARAMETERS

When **Inlet** is selected as the **Flow direction**, the **Input pressure** p_{input} defines the pressure at the fan inlet.

When **Outlet** is selected as the **Flow direction**, the **Exit pressure** p_{exit} defines the pressure at the fan outlet.

When **Include gravity** is selected and **Use reduced pressure** is not selected in the interface's **Physical model** section, the **Compensate for hydrostatic pressure** (named **Compensate for hydrostatic pressure approximation** for weakly compressible or compressible flow) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{input} or p_{exit} user input.

For either flow direction, **Flow condition** specifies a static pressure curve — **linear**, **data**, or **user defined**.

Static Pressure Curve, Linear

For both **Inlet** and **Outlet** flow directions, if **Linear** is selected, values or expressions for the **Static pressure at no flow** p_{nf} and the **Free delivery flux** $V_{0,\text{fd}}$ should be specified. The static pressure curve is equal to the static pressure at no flow when $V_0 < 0$ and equal to 0 when the fluxis larger than the free delivery flux.

Static Pressure Curve, Data

The **Static pressure curve data** can be entered or loaded under the **Static Pressure Curve Data** section that displays for this option. The interpolation between points given in the table is defined using the **Interpolation function type** list in the **Static Pressure Curve Interpolation** section.

Static Pressure Curve, User Defined

With the **Static pressure curve, user defined** option, a different value or expression for the **Fan flux interpolation function** can be specified. The flux across the selection where this boundary condition is applied is defined by *phys_id*`.V0` where *phys_id* is the name (for example, *phys_id* is `spf` by default for laminar single-phase flow). In order to avoid unexpected behavior, the function used for the fan curve returns the maximum of the user-defined function and 0.

UNITS

This section is available when **Static pressure curve, data** is selected as the **Flow condition**. Units can be specified for the **Flux** and **Static pressure**.

STATIC PRESSURE CURVE DATA

When **Static pressure curve, data** is selected as the **Flow condition**, a table appears, where values or expressions the **Flux** and **Static pressure** can be specified or imported from a text file by clicking the **Load from file** button ( ) under the table. Units can be specified for the **Flux** and the **Static pressure curve**.

STATIC PRESSURE CURVE INTERPOLATION

This section is available when **Static pressure curve, data** is selected as the **Flow condition**. The available options for the **Interpolation function type** are **Linear**, **Piecewise cubic**, and **Cubic spline**.

The extrapolation method always returns a constant value. In order to avoid problems with undefined data, the function used for the boundary condition returns the maximum of the interpolated function and 0.

TURBULENCE CONDITIONS ON FAN OUTLET

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε, specific dissipation rate, ω, or turbulent relative fluctuations, ζ, the values of the **Turbulent kinetic energy**, **Turbulent relative fluctuations** (for the v2-f turbulence model) and the **Turbulent dissipation rate** or **Specific dissipation rate** on the downstream side of the fan should be specified. If **Include transition modeling** is active for the SST turbulence model, the option to specify **Intermittency** is also available. Alternatively, the **Reference velocity scale** can be used to specify default values.

Fan and Grille Boundary Conditions

The **Fan** feature uses the flux across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several fans on boundaries that are not connected, it is good practice to use different Fan or Interior Fan features with connected boundaries.

Interior Fan

The **Interior Fan** condition represents interior boundaries where a fan condition is set using a fan pressure curve to avoid an explicit representation of the fan. The **Interior Fan** defines a boundary condition on a slit for laminar flow. That means that the pressure and the velocity can be discontinuous across this boundary.

One side represents a flow inlet; the other side represents the fan outlet. The fan boundary condition ensures that the mass flow rate is conserved between its inlet and outlet:

$$\int_{\text{inlet}} \rho \mathbf{u} \cdot \mathbf{n} + \int_{\text{outlet}} \rho \mathbf{u} \cdot \mathbf{n} = 0$$

This boundary condition acts like a Pressure Conditions boundary condition on each side of the fan. When a pressure curve is used, the pressure at the fan outlet is fixed so that the mass flow rate is conserved. On the fan inlet the pressure is set to the pressure at the fan outlet minus the pressure drop induced by the fan. The pressure drop is defined from the static pressure curve, and is usually a function of the flux. When the flux is prescribed the pressure at the inlet and at the outlet are set so that the flux obtains the desired value.

To define a fan boundary condition on an exterior boundary, the Fan condition should be used instead.

FLOW DIRECTION

The **Flow direction** can be defined by selecting **Along normal vector** or **Opposite to normal vector**. This defines which side of the boundary is the fan's inlet and which side is the fan's outlet.

Select **Prescribe flow direction**, to enforce the flow direction of the fluid when it enters the domain located at the fan outlet.

- For **Normal flow** it sets the tangential velocity component to zero.
- For **Swirl flow** (which is available for 3D or 2D axisymmetric when the **Swirl flow** checkbox in the **Physical Model** section is selected) it specifies a swirl flow on the downstream side of the fan based on the **Rotation axis base point** $\mathbf{r}_{\text{bp}}$, **Revolutions per time** f, **Rotational direction**, and **Swirl ratio** c_{sf}.
- For **User defined** an **Inflow velocity direction** $\mathbf{d}_{\mathbf{u}}$ (dimensionless) should be specified. The magnitude of $\mathbf{d}_{\mathbf{u}}$ does not matter, only the direction. $\mathbf{d}_{\mathbf{u}}$ must point into the domain.

PARAMETERS

All the settings for this section except **Prescribe flux** are the same as for the Fan node. See Static Pressure Curve, Linear and Static Pressure Curve, Data for details.

When **Prescribe flux** is selected, define the **Prescribed flux** $V_{0,\text{pf}}$ (SI unit m^3/s, default value 0.01 m^3/s).

TURBULENCE CONDITIONS ON FAN OUTLET

When the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε, specific dissipation rate, ω, or turbulent relative fluctuations, ζ, the values of the **Turbulent kinetic energy**, **Turbulent relative fluctuations** (for the v2-f turbulence model) and the **Turbulent dissipation rate** or **Specific dissipation rate** on the downstream side of the fan should be specified. If **Include transition modeling** is active for the SST turbulence model, the option to specify **Intermittency** is also available. Alternatively, the **Reference velocity scale** can be used to specify default values.

After a boundary has been selected, an arrow displays in the **Graphics** window to indicate the selected flow direction. If the selection changes, the arrow can be updated by clicking any node in the **Model Builder** and then clicking the **Interior fan** node again to update the **Graphics** window.

Fan Defined on an Interior Boundary

The **Interior Fan** feature uses the flux across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several fans on boundaries that are not connected, it is good practice to use different Fan or Interior Fan features with connected boundaries.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities (velocity, pressure, and turbulence variables) across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-slip conditions on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed. It is compatible with laminar and turbulent flow.

BOUNDARY CONDITION

The following **Boundary condition** options are available.

No Slip

The **No slip** condition models solid walls. No slip walls are walls where the fluid velocity relative to the wall is zero. For an interior stationary wall this means that $\mathbf{u} = 0$ on both sides of the wall.

For turbulent flows, the no slip conditions may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall Treatment** is set to **Wall functions**, the **Apply wall roughness** option becomes available. When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. Select **Generic roughness** in order to specify more general roughness types.

- For **Sand roughness** an **Equivalent sand roughness height** k_{seq} should be specified.
- For **Generic roughness** a **Roughness height** k_{s} and a dimensionless **Roughness parameter** C_{s} should be specified.

Slip

The **Slip** condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It implicitly assumes that there are no viscous effects on either side of the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the important effect is to prevent the exchange of fluid between the regions separated by the interior wall.

Navier Slip

The **Navier slip** condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{\mathrm{wall}} = 0$, and adds a tangential stress on each side of the wall

$$\mathbf{K}_{\mathrm{nt}} = -\frac{\mu}{\beta}\mathbf{u}_{\mathrm{slip}}$$

where β is a slip length. For more information, see the **Navier Slip** option in the Wall feature.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{\mathbf{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model

component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Zero (Fixed wall)** from **Translational velocity** selection list to prescribe $\mathbf{u}_{\mathrm{tr}} = \mathbf{0}$.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**. The **Constraints** settings can be set to **Automatic**, **Pointwise constraints**, or **Nitsche constraints**. **Mixed constraints** can be selected when imposing a no slip condition exactly.

- Wall
- The Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Grille

The **Grille** boundary condition models the pressure drop caused by having a grille that covers the inlet or outlet.

PARAMETERS

When **Inlet** is selected as the **Flow direction**, the **Input pressure** p_{input} defines the pressure at the fan inlet.

When **Outlet** is selected as the **Flow direction**, the **Exit pressure** p_{exit} defines the pressure at the fan outlet.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{input} or p_{exit} user input.

When **Quadratic loss** is selected for the **Static pressure curve**, the **Quadratic loss coefficient** qlc should be specified. qlc defines the static pressure curve which is a piecewise quadratic function equal to 0 when the flow rate is < 0, equal to $V_0^2 \cdot$qlc when the flow rate is > 0. Alternately, when **Loss coefficient** K is specified for the **Static pressure curve**, a pressure drop equal to $0.5K\rho(\mathbf{u} \cdot \mathbf{n})^2$ is prescribed. See Fan for other settings for the Laminar Flow interface. Note that for the Turbulent Flow interfaces, **Quadratic loss** and **Loss coefficient** are the only available options for **Static pressure curve**.

TURBULENCE CONDITIONS

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε, specific dissipation rate, ω, or turbulent relative fluctuations, ζ, the **Specify turbulent length scale and intensity** and **Specify turbulence variables** options are available for the turbulence conditions on the downstream side of the grille. If **Include transition modeling** is active for the SST turbulence model, the option to specify **Intermittency** is also available. Alternatively, the **Reference velocity scale** can be used to specify default values.

Fan and Grille Boundary Conditions

The **Grille** feature uses the flow rate across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several grilles on boundaries that are not connected, it is good practice to use different Grille features with connected boundaries.

Porous Interface

The **Porous Interface** condition is designed to properly account for a sudden jump in porosity, ε_p, across a boundary between different domains. It describes possible discontinuity of stress across the interface, and also reveals modified behavior of tangential velocity due to boundary layer on the upstream side of the interface. Choose among the following options under the **Continuity conditions**:

- **Velocity and stress** — stress continuity is invoked;

- **Velocity and porosity-corrected stress** (default)— the sum of stress and a contribution due to the inertial term being constant across the interface;
- **Velocity and porosity-corrected stress with loss** — the sum of the stress and a contribution due to the inertial term is lost in the downstream direction.

All three options give continuity of the velocity across the interface in constant-density flows, while in case of a jump in density:

1. give continuity of the mass flux (product of density and normal velocity) and tangential velocity;
2. account for the density-jump correction in the stress condition.

When **Velocity and porosity-corrected stress with loss** is chosen, a **Pressure loss model** needs to be specified. The options are:

- **User-defined loss coefficients** (default). Enter values for **Expansion loss coefficient** and **Contraction loss coefficient**;
- **Borda–Carnot**. Specify **Vena contracta model**.

Vena contracta model allows two options:

- **User defined** (default) — enter value of **Vena contracta coefficient**;
- **Weisbach** — enter values of **Lower limit** and **Exponent**.

Notice that the notions 'expansion' and 'contraction' used in this section correspond not to geometrical changes, but to the variations of the microscopic structure across the interface in the flow direction — increasing or decreasing porosity, ε_p, respectively.

Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the Wall node is used as fallback unless another feature has been selected for the boundary.

The **Wall** fallback condition is incompatible with the **Low Re** wall treatment for the k-ω, SST and Low Reynolds number k-ε turbulence models when the overlapping parts of the pair changes with time. For nonchanging overlaps it can be made compatible by

selecting **Nonpair region** from **Allowed region** under **Applicable Pair Region** in the **Settings** window for the **Wall** feature.

When the condition is set for pairs adjacent to domains with different porosity ε_p, it imposes conditions identical to the **Porous Interface** feature, which is designed to properly account for a sudden jump in porosity. See the section Porous Interface above for further details (note that the **Flow Continuity** does not account for the density-jump corrections),

About Pairs

Pressure Point Constraint

The **Pressure Point Constraint** condition can be used to specify the pressure level. If it is not possible to specify the pressure level using a boundary condition, the pressure level must be set in some other way, for example, by specifying a fixed pressure at a point.

PRESSURE CONSTRAINT

The relative pressure value is set by specifying the **Pressure** p_0. If the reference pressure p_{ref} defined at the physics interface level is equal to zero, p_0 represents the absolute pressure.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for incompressible flows) checkbox is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

The **Apply reaction terms on** setting is set per default to **Individual dependent variables**. **All physics (symmetric)** cannot be used together with a segregated solver when fluid flow is coupled with Moving Mesh, Level Set, or Phase Field in Fluids.

Point Mass Source

This feature requires at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Point Mass Source** feature models mass flow originating from an infinitely small domain centered around a point.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, there are two nodes: one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

SOURCE STRENGTH

The source **Mass flux**, $\dot{q}_p$ should be specified. A positive value results in mass being ejected from the point into the computational domain. A negative value results in mass being removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that a point source located on a symmetry plane has twice the given strength.

Mass Sources for Fluid Flow in the *COMSOL Multiphysics Reference Manual*

Line Mass Source

This feature requires at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Line Mass Source** feature models mass flow originating from a tube region with infinitely small radius.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, there are two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the axis of symmetry
3D	Edges

SOURCE STRENGTH

The source **Mass flux**, $\dot{q}_1$, should be specified. A positive value results in mass being ejected from the line into the computational domain and a negative value means that mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This, for example, has the effect that a line source located on a symmetry plane has twice the given strength.

Mass Sources for Fluid Flow in the *COMSOL Multiphysics Reference Manual*

Generate New Turbulence Model Interface

This global feature requires a CFD Module license. It can be used to create a new turbulent flow interface based on the current laminar or turbulent flow interface. The new interface inherits the property values from the original interface except for the turbulence related ones. All the features in the original interface are also inherited by the newly created interface except for the **Generate New Turbulence Model Interface** feature itself and the **Initial Values** feature. The initial values of the new interface are either default values or estimates from the solution of the original interface depending on the settings in the **Generate New Turbulence Model Interface** feature. Note that the parameters and expressions in text fields in all the features, except for **Initial Values** and the **Name** column in **Global Equation**, get exactly the same expressions as in the original model. Therefore, any dependencies on expressions or dependent variables from the physics interface must be reviewed and updated manually if necessary.

MODEL GENERATION

This section contains a Boolean input, **Copy only active settings**, which is selected by default. When selected, the disabled features and settings in the original model are not transferred to the new interface.

The **Create** button generates the new interface.

TURBULENCE MODEL INTERFACE

All available turbulence models can be selected from the list:

- Turbulent Flow, k-ε
- Turbulent Flow, Algebraic yPlus
- Turbulent Flow, L-VEL
- Turbulent Flow, k-ω
- Turbulent Flow, SST
- Turbulent Flow, Low Reynolds number k-ε
- Turbulent Flow, Spalart–Allmaras
- Turbulent Flow, v^2-f
- Turbulent Flow, Wilcox R-ω
- Turbulent Flow, SSG-LRR

STUDY

The **Study** section contains two lists: **Study type** and **Initial value from study**. When Turbulent Flow, k-ε or Turbulent Flow, k-ω is selected as the **Turbulence Model Interface**, the **Study type** contains the following two options:

- **Stationary**
- **Time-dependent**

The default value is **Stationary**. For all other turbulence models, the available **Study type** options are:

- **Stationary with initialization**
- **Time dependent with initialization**

with default value **Stationary with initialization**. Note that the created new study only solves for the new turbulence interface.

Initial value from study contains a list of the studies that are currently in the model. It can also be set to **None**. If there is no study available, the default option is **None**. If there are available studies, the first study is the default option.

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value. When a turbulence model that solves for the turbulent kinetic energy, k, is used, the option **Include buoyancy-induced turbulence** is available. When selected, the **Buoyancy contribution** is by default set to **Automatic from multiphysics**. Contributions are only obtained from multiphysics couplings that support buoyancy-induced turbulence, such as Nonisothermal Flow. If the **Buoyancy contribution** is switched to **User defined**, a text field for the **Turbulent Schmidt number** appears. See also Theory for Buoyancy-Induced Turbulence in the *CFD Module User's Guide*.

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{const}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{const}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

The Rotating Machinery, Laminar and Turbulent Flow Interfaces

The **Rotating Machinery, Laminar Flow (spf)** and **Rotating Machinery, Turbulent Flow (spf)** interfaces, found under the **Single-Phase Flow** > **Rotating Machinery** branch ( ) when adding a physics interface, are used for modeling flow where one or more of the boundaries rotate in a periodic fashion. This is used for mixers and propellers.

The physics interfaces support compressible, weakly compressible and incompressible flow, the flow of non-Newtonian fluids described by the Power Law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models, as well as turbulent flow. In addition, the physics interfaces support creeping flow, although the shallow channel approximation is redundant.

In this section:

- Moving Mesh
- The Rotating Machinery, Laminar Flow Interface
- The Rotating Machinery, Turbulent Flow, Algebraic yPlus Interface
- The Rotating Machinery, Turbulent Flow, L-VEL Interface
- The Rotating Machinery, Turbulent Flow, k-ε Interface
- Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces

Moving Mesh

The Rotating Machinery, Fluid Flow interfaces rely on ALE (arbitrary Lagrangian–Eulerian) moving mesh functionality for their rotating domain and free surface implementation.

ROTATING DOMAINS

When a **Rotating Machinery, Fluid Flow** interface is added using the **Model Wizard**, a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** > **Moving Mesh** node. It contains settings for specifying the rotation of one or several domains. By default, **All domains** are selected. Under the **Rotating Domain**, you can exclude any nonrotating fluid domains. For both 3D and 2D components, the **Rotation type** should be set to **Specified rotational velocity**.

Select a **Rotational velocity expression** — **General revolutions per time** (the default), **Constant revolutions per time**, **General angular velocity**, or **Constant angular velocity**.

- For **Constant revolutions per time** or **General revolutions per time**, enter a value or expression respectively in the **Revolutions per time** input field and optionally an **Initial angle**. The angular velocity in this case is defined as the input multiplied by 2π.
- For **Constant angular velocity** or **General angular velocity** enter a value or an expression respectively in the **Angular velocity** input field and optionally an **Initial angle**.

3D Components

For 3D components, select the **Rotation axis base point**, $\mathbf{r}_{ax}$. The default is the origin. Select the **Rotation axis**, $\mathbf{u}_{rot}$, the z-axis is the default. If the x-axis is selected, it corresponds to a rotational axis $(1, 0, 0)$ with the origin as the base point, and correspondingly for the y-axis and z-axis.

2D Components

For 2D components, enter coordinates for the **Rotation axis base point**, $\mathbf{r}_{ax}$. The default is the origin $(0, 0)$.

The Rotating Machinery, Laminar Flow Interface

The **Rotating Machinery, Laminar Flow (spf)** interface ( ), found under the **Single-Phase Flow** > **Rotating Machinery** branch ( ), is used to simulate flow at low to moderate Reynolds numbers in geometries with one or more rotating parts. The physics interface supports incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3). It also supports modeling of non-Newtonian fluids. The physics interface is available for 3D and 2D components.

There are two study types available for this physics interface. Using the **Time Dependent** study type, rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and rotation is accounted for by the inclusion of centrifugal and Coriolis forces. In both types, the momentum balance is governed by the Navier–Stokes equations, and the mass conservation is governed by the continuity equation. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** under **Laminar Flow** — **Fluid Properties**, **Wall**, and **Initial Values**. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** node. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also

right-click **Laminar Flow** to select physics features from the context menu. See Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

	Pseudo Time Stepping for Laminar Flow Models

	Laminar Flow in a Baffled Stirred Mixer: Application Library path **CFD_Module/Fluid-Structure_Interaction/baffled_mixer**

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `spf`.

In addition to the settings described below, see The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces for all the other settings available. See Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces for links to all the physics nodes.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Pseudo Time Stepping

Select the **Use pseudo time stepping for stationary equation form** checkbox to add pseudo time derivatives to the equation when the **Frozen Rotor** equation form is used. (Frozen rotor is a pseudo stationary formulation.) When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable `CFLCMP` which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** $\mathrm{CFL}_{\mathrm{loc}}$ (dimensionless).

The Rotating Machinery, Turbulent Flow, Algebraic yPlus Interface

The **Rotating Machinery, Turbulent Flow, Algebraic yPlus (spf)** interface (), found under the **Single-Phase Flow** > **Rotating Machinery** branch () when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Algebraic yPlus interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled wall distance. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

Two study types are available for this physics interface. Using the **Time Dependent with Initialization** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor with Initialization** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. Both study types includes an initial Wall Distance Initialization step in order to compute the wall distance. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder** under **Turbulent Flow, Algebraic yPlus** — **Fluid Properties**, **Wall**, and **Initial Values**. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** node. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Turbulent Flow, Algebraic yPlus** to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the settings below, see the advanced settings for The Rotating Machinery, Laminar Flow Interface, and The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces.

TURBULENCE MODEL PARAMETERS

The turbulence model parameters for the Algebraic yPlus model, κ_a and B_a, have been optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$
- **Pressure** p
- **Reciprocal wall distance** G
- **Wall distance in viscous units** yPlus (dimensionless)

The Rotating Machinery, Turbulent Flow, L-VEL Interface

The **Rotating Machinery, Turbulent Flow, L-VEL (spf)** interface (), found under the **Single-Phase Flow** > **Rotating Machinery** branch () when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, L-VEL interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled fluid flow velocity tangential to the nearest wall. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

Two study types available for this physics interface. Using the **Time Dependent with Initialization** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor with Initialization** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. Both study types includes an initial Wall Distance Initialization step in order to compute the wall distance. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder** under **Turbulent Flow, L-VEL** — **Fluid Properties**, **Wall**, and **Initial Values**. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** node. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Turbulent Flow, L-VEL** to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the interface settings defined below, see the advanced settings for The Rotating Machinery, Laminar Flow Interface, and the settings in The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces.

TURBULENCE MODEL PARAMETERS

The turbulence model parameters for the L-VEL model, κ_l and E_l, have been optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$
- **Pressure** p
- **Reciprocal wall distance** G
- **Tangential velocity in viscous units** uPlus (dimensionless)

The Rotating Machinery, Turbulent Flow, k-ε Interface

The **Rotating Machinery, Turbulent Flow, k-ε (spf)** interface (), found under the **Single-Phase Flow** > **Rotating Machinery** branch () when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3).

The momentum balance is governed by the Navier–Stokes equations, and the mass conservation is governed by the continuity equation. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

There are two study types available for this physics interface. Using the **Time Dependent** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder** under **Turbulent Flow, k-ε** — **Fluid Properties**, **Wall**, and **Initial Values**. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model**

Builder under the **Definitions** node. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Turbulent Flow, k-ε** to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the defined settings below, see the advanced settings for The Rotating Machinery, Laminar Flow Interface, and the settings in The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1}, C_{e2}, C_{μ}, σ_{k}, σ_{e}, κ_{v}, and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p
- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep

Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces

All versions of the Rotating Machinery, Fluid Flow interfaces use the following domain, boundary, point, and pair physics nodes.

- Contact Angle
- Stationary Free Surface

The nodes are available under the option **Rotating Machinery** from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

The following nodes, available in the Fluid Flow interfaces, are described for the Laminar Flow interface:

- Boundary Stress
- Initial Values
- Interior Wall
- Flow Continuity
- Fluid Properties
- Inlet
- Line Mass Source
- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Screen
- Symmetry
- Volume Force
- Wall

Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

Stationary Free Surface

This postprocessing feature is used to estimate the deformation of a free surface from the pressure distribution on the boundary when using the **Frozen Rotor** or **Frozen Rotor with Initialization** study types. When computing the flow field, a slip condition together with a constant pressure level p_{ext} is applied on the boundary. The free surface deformation η_{FS} is evaluated from the linearized free surface condition in a separate study step, Wall Distance Initialization, using the pressure from the Frozen Rotor study step:

$$p(\mathbf{x}_0) - p_{\text{ext}} + \hat{\mathbf{n}} \cdot \nabla p\big|_{\mathbf{x}=\mathbf{x}_0} \eta_{\text{FS}} = -\sigma \nabla_S^2 \eta_{\text{FS}} \tag{3-10}$$

Here, σ is the surface tension coefficient, $\mathbf{x} = \mathbf{x}_0$ represents the position of the undisturbed surface (the feature selection), and $\hat{\mathbf{n}}$ is its unit normal. The correct study sequence can be triggered by toggling the study window once a selection for the Stationary Free Surface feature has been made.

The Stationary Free Surface feature is supported by laminar and turbulent flow, and is applicable for small surface deformations (η_{FS} and its gradient should be small

compared to the dimensions of the computational domain). If the surface deformation is large, a time-dependent study with a **Deforming Domain** and a Free Surface feature should be used instead.

Iterative solvers are necessary to reduce the cost of models with large number of degrees of freedom. The fluid flow interfaces use a **Smoothed aggregation AMG** solver per default. When the Stationary Free Surface feature is active and has a nonempty selection in a frozen rotor or stationary study step, a **Geometric multigrid** solver is used instead to ensure robustness of the model.

	The Choice of Solver and Solver Settings in the *CFD Module User's Guide* and Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

STATIONARY FREE SURFACE

Enter an **External pressure** p_{ext} corresponding to the average pressure level on the free surface.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation.

The **Surface tension coefficient** σ (SI unit: N/m) can be specified from predefined libraries, by selecting **Library coefficient, liquid/gas interface** (the default) or **Library coefficient, liquid/liquid interface**, or be set to **User defined**.

- For **Library coefficient, liquid/gas interface** select an option from the list — **Water/Air** (the default), **Acetone/Air**, **Acetic acid/Air**, **Ethanol/Air**, **Ethylene glycol/Ethylene glycol vapor**, **Diethyl ether/Air**, **Glycerol/Air**, **Heptane/Nitrogen**, **Mercury/Mercury vapor**, or **Toluene/Air**.
- For **Library coefficient, liquid/liquid interface** select an option from the list — **Benzene/Water, 20°C**, **Corn oil/Water, 20°C**, **Ether/Water, 20°C**, **Hexane/Water, 20°C**, **Mercury/Water, 20°C**, or **Olive oil/Water, 20°C**.

Only one Stationary Free Surface feature can be applied in a Rotating Machinery, Fluid Flow interface, and it requires the study to be stationary (Frozen Rotor).

Contact Angle

This feature specifies the contact angle between the free surface and a solid wall.The Contact Angle feature is a subfeature to, and added under a Stationary Free Surface feature. See the Contact Angle feature in the Multiphase Flow Interfaces chapter.

The Viscoelastic Flow Interface

The **Viscoelastic Flow (vef)** interface ( ) is used for simulating single-phase flows of viscoelastic fluids. The physics interface is only suitable for incompressible flows.

The equations solved by the Viscoelastic Flow interface are the continuity equation for conservation of mass, the Navier–Stokes equations, augmented by an elastic stress tensor term, and a constitutive equation that defines the extra elastic stress contribution.

The Viscoelastic Flow interface is available for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes equations, continuity equations, and the constitutive relations between the extra elastic stress term and the velocity gradient. The Fluid Properties feature provides an interface for defining the fluid material and its properties. Viscoelastic, Newtonian, and Inelastic non-Newtonian constitutive relations are available. The boundary conditions are essentially the same as for the Laminar Flow interface. When this physics interface is added, the following default nodes are also added in the **Model Builder**:

- **Fluid Properties**
- **Initial Values**
- **Wall**

Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Viscoelastic Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is vef.

PHYSICAL MODEL

This node specifies the properties of the Viscoelastic Flow interface, which describe the overall type of fluid flow model.

Include Gravity

When the **Include gravity** checkbox is selected, a global **Gravity** feature is shown in the interface model tree.

Also, when the **Include gravity** checkbox is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. For more information, see Gravity.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- **Velocity field** $\mathbf{u}$ and its components
- **Pressure** p

If the **Viscoelastic** constitutive relation is selected, the **Fluid Properties** node also adds as variables the components of the elastic stress tensor.

For all other settings, see The Laminar Flow Interface.

- Domain, Boundary, Point, and Pair Nodes for the Viscoelastic Interface
- Theory for the Viscoelastic Flow Interface

Flow of Viscoelastic Fluid Past a Cylinder: Application Library path **CFD_Module/Single-Phase_Flow/cylinder_flow_viscoelastic**

Domain, Boundary, Point, and Pair Nodes for the Viscoelastic Interface

For the Viscoelastic Flow interface the Fluid Properties node is described in this section.

The following nodes (listed in alphabetical order) are described in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow:

- Boundary Stress
- Flow Continuity
- Free Surface
- Fluid-Fluid Interface
- Gravity
- Initial Values
- Inlet
- Interior Wall
- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Volume Force
- Wall

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations solved by the physics interface. For the viscoelastic fluids, the constitutive relations for the extra elastic stress tensor are also added. The node also provides an interface for defining the material properties of the fluid.

Except where included below, see Fluid Properties for all the other settings.

Constitutive Relation

Viscoelastic (default), **Specify dynamic viscosity** and **Inelastic non-Newtonian** options are available. If **Viscoelastic** constitutive relation is selected, the **Fluid Properties** node also adds the viscoelastic variables and equations.

For **Viscoelastic** constitutive relation, specify **Solvent viscosity** μ_s and select a **Material model** — **Oldroyd-B**, **Giesekus**, or **FENE-P**. Viscoelastic material can be described as consisting of one or more branches. For each viscoelastic branch, enter parameters in the table. See the setting for each viscoelastic model that follows.

Oldroyd-B

For **Oldroyd-B** enter the model parameters in the table. In each **Branch** raw enter the polymer viscosity μ_{em} in the **Viscosity** column, and the relaxation time λ_{em} in the **Relaxation time** column.

Giesekus

For **Giesekus**, in each **Branch** raw enter the polymer viscosity μ_{em} in the **Viscosity** column, the relaxation time λ_{em} in the **Relaxation time** column, and the mobility factor α_{em} in the **Mobility** column.

FENE-P

For **FENE-P**, in each **Branch** raw enter the polymer viscosity μ_{em} in the **Viscosity** column, the relaxation time λ_{em} in the **Relaxation time** column, and the extensibility parameter L_{em} in the **Extensibility** column.

- Use the **Add** button (+) to add a row to the table and the **Delete** button ( ) to delete a row in the table.
- Use the **Load from file** button ( ) and the **Save to file** button ( ) to load and store data for the branches in a text file with three space-separated columns.

DISCRETIZATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Select shape function type for the components of the auxiliary viscoelastic tensor. The default setting is **Linear**.

INITIAL VALUES

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Enter initial values or expressions for the components of the auxiliary viscoelastic tensor. The initial values can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver. Note, that if several branches are specified, the initial values entered above are applied to all branches.

Note: The **Interior Walls** boundary condition and Pair conditions are not applicable on the boundaries that are adjacent to the Fluid properties nodes with different number of branches.

The Potential Flow Interfaces

In this section

- The Incompressible Potential Flow Interface
- The Compressible Potential Flow Interface (in the *Acoustics Module User's Guide*)

The Incompressible Potential Flow Interface

The **Incompressible Potential Flow (ipf)** interface ( ) is used for simulating irrotational, inviscid, and incompressible flow. The main application of the interface is to provide initial solutions for other Single-Phase Flow interfaces.

The equation solved by the Incompressible Potential Flow interface is the Laplace equation for a velocity potential. This can be used to derive both a velocity and static pressure.

The Incompressible Potential Flow interface is available for stationary analyses. The main feature is Fluid Properties, which adds the Laplace equation. The Fluid Properties feature provides an interface for defining the fluid material and its properties used to derive the velocity and pressure. When this physics interface is added, the following default nodes are also added in the **Model Builder**:

- **Fluid Properties**
- **Initial Values**
- **Wall**

Then, from the **Physics** toolbar, add other nodes that implement boundary conditions. You can also right-click **Incompressible Potential Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is ipf.

PRESSURE

This node specifies **Total pressure** (SI unit: Pa) used to compute the pointwise static pressure from the potential flow solution.

DEPENDENT VARIABLES

This physics interface solves for the **Velocity Potential** ϕ-dependent variable (field).

If required, the names of the field, component, and dependent variable can be edited. Editing the name of a scalar dependent variable changes both its field name and the dependent variable name. If a new field name coincides with the name of another field of the same type, the fields share degrees of freedom and dependent variable names. A new field name must not coincide with the name of a field of another type or with a component name belonging to some other field. Component names must be unique within a model except when two fields share a common field name.

DISCRETIZATION

Select shape function type for the velocity potential. The default setting is **Quadratic**.

- Domain, Boundary, Point, and Pair Nodes for the Viscoelastic Interface
- Theory for the Incompressible Potential Flow Interface

Flow Around an Inclined NACA 0012 Airfoil: Application Library path **CFD_Module/Verification_Examples/naca0012_airfoil**

Domain, Boundary, Point, and Pair Nodes for the Incompressible Potential Flow Interface

The Incompressible Potential Flow Interface has the following domain, boundary, and pair nodes:

- Initial Values
- Interior Wall
- Flow Continuity
- Fluid Properties
- Open Boundary
- Periodic Flow Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Potential Point Constraint
- Symmetry
- Velocity
- Wall

[1] Described for the Laminar Flow interface.

Boundary conditions for axial symmetry boundaries are not required. For the symmetry axis at $r = 0$, the software automatically provides a suitable boundary condition and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

The **Fluid Properties** node adds the Laplace equation solved by the physics interface. The node also provides an interface for defining the density of the fluid, and builds the velocity and static pressure.

Material Properties

The density can either be specified by a material, or by a **User defined** expression.

Initial Values

Use the **Initial Values** node to define the initial values of the velocity potential variable.

INITIAL VALUES

An initial value or expression should be specified for the **Velocity Potential** ϕ.

Wall

The **Wall** node sets a slip wall condition for the fluid. This prescribes a no-penetration condition, $\mathbf{u}\cdot\mathbf{n} = 0$.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Normal wall velocity** setting controls the normal wall velocity U_{bnd}. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $U_{bnd} = 0$. If the frame moves, U_{bnd} becomes equal to the frame movement projected on the wall normal. U_{bnd} is accounted for in the actual nonpenetration boundary condition prescribed, so that $\mathbf{u} \cdot \mathbf{n} = U_{bnd}$.

Select **Zero (Fixed wall)** from **Normal wall velocity** selection list to always prescribe $U_{bnd} = 0$.

Velocity

The **Velocity** node sets a normal inflow velocity condition for the fluid. This prescribes a flux condition for the velocity potential, $\nabla\phi \cdot \mathbf{n} = -U_{in}$.

Open Boundary

The **Open Boundary** node sets a normal flow condition for the fluid. The level of ϕ is set to a constant value along the boundary, so that the tangential derivative of ϕ is zero.

OPEN BOUNDARY

The potential level is set by specifying the **Velocity potential** ϕ_{bnd}.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

Symmetry

The **Symmetry** node prescribes a symmetry condition for the velocity potential, $\nabla\phi \cdot \mathbf{n} = 0$.

Potential Point Constraint

The **Potential Point Constraint** node can be used to specify the velocity potential level. If it is not possible to specify the velocity potential level using a boundary condition, the level must be set in some other way, such as specifying a fixed potential at a point.

POTENTIAL POINT CONSTRAINT

The potential level is set by specifying the **Velocity potential** ϕ_p.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group (the **Destination Selection** section is optional). Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

OFFSET

The **Offset** at the boundary specifies a value or expression for either the **Velocity potential difference**, $\phi_{src} = -\phi_{dst}$. The offset ensures a gradient of the Velocity potential between the source and destination, so that the velocity is nonzero.

BOUNDARY SELECTION

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

The software usually automatically identifies the boundaries as either source boundaries or destination boundaries, as indicated in the selection list. This works fine for cases like opposing parallel boundaries. In other cases, right-click **Periodic Flow Condition** and select **Manual Destination Selection** to control the destination. By default it contains the selection that COMSOL Multiphysics identifies.

DESTINATION SELECTION

This section is available for specifying the destination boundaries, if needed, when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Flow Condition** node. You can only select destination boundaries from the union of all source and destination boundaries.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping**

Between Source and Destination section, see Mapping Between Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall node available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the velocity potential across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = U_{bnd}$, on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Normal wall velocity** setting controls the normal wall velocity U_{bnd}. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $U_{bnd} = 0$. If the frame moves, U_{bnd} becomes equal to the frame movement projected on the wall normal. U_{bnd} is accounted for in the actual no-penetration boundary condition prescribed, so that $\mathbf{u} \cdot \mathbf{n} = U_{bnd}$.

Select **Zero (Fixed wall)** from **Normal wall velocity** selection list to always prescribe $U_{bnd} = 0$.

Flow Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the velocity potential variable is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts.

By default, the Wall node is used as fallback unless another feature has been selected for the boundary.

About Pairs

LOCATION IN USER INTERFACE

Right-click the physics interface and select **Pairs** > **Continuity**.

Ribbon

Physics tab with the physics interface selected:

Pairs > **Continuity**

Theory for the Single-Phase Flow Interfaces

Also see Theory for the Turbulent Flow Interfaces and Theory for the Rotating Machinery Interfaces.

The theory for the Single-Phase Flow, Laminar Flow interface is described in this section:

- General Single-Phase Flow Theory
- Compressible Flow
- Weakly Compressible Flow
- The Mach Number Limit
- Incompressible Flow
- The Reynolds Number
- Non-Newtonian Flow
- Gravity
- The Boussinesq Approximation
- Theory for the Wall Boundary Condition
- Prescribing Inlet and Outlet Conditions
- Mass Flow
- Fully Developed Flow (Inlet)
- Fully Developed Flow (Outlet)
- No Viscous Stress
- Normal Stress Boundary Condition
- Vacuum Pump Boundary Condition
- Fan Defined on an Interior Boundary
- Fan and Grille Boundary Conditions
- Screen Boundary Condition
- Porous Interface
- Mass Sources for Fluid Flow

- Numerical Stability — Stabilization Techniques for Fluid Flow
- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- Nitsche Constraints
- Particle Tracing in Fluid Flow
- References for the Single-Phase Flow, Laminar Flow Interfaces

The theory about most boundary conditions is found in Ref. 2.

General Single-Phase Flow Theory

The Single-Phase Fluid Flow interfaces are based on the Navier–Stokes equations, which in their most general form read

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-11}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F} \tag{3-12}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T \right) = -(\nabla \cdot \mathbf{q}) + \mathbf{K}:\mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T}\bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p \right) + Q \tag{3-13}$$

where

- ρ is the density (SI unit: $\mathrm{kg/m^3}$)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is pressure (SI unit: Pa)
- $\mathbf{I}$ is the identity matrix (unitless)
- $\mathbf{K}$ is the viscous stress tensor (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: $\mathrm{N/m^3}$)
- C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- $\mathbf{q}$ is the heat flux vector (SI unit: $\mathrm{W/m^2}$)

- Q contains the heat sources (SI unit: W/m^3)
- $\mathbf{S}$ is the strain-rate tensor:

$$\mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

The operation ":" denotes a contraction between tensors defined by

$$\mathbf{a}:\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm} \tag{3-14}$$

This is sometimes referred to as the double dot product.

Equation 3-11 is the continuity equation and represents conservation of mass. Equation 3-12 is a vector equation which represents conservation of momentum. Equation 3-13 describes the conservation of energy, formulated in terms of temperature. This is an intuitive formulation that facilitates boundary condition specifications.

To close the equation system, Equation 3-11 through Equation 3-13, constitutive relations are needed.

For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

$$\mathbf{K} = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \tag{3-15}$$

The dynamic viscosity, μ (SI unit: Pa·s), for a Newtonian fluid is allowed to depend on the thermodynamic state but not on the velocity field. All gases and many liquids can be considered Newtonian.

For an inelastic non-Newtonian fluid, the relationship between stress and strain rate is nonlinear, and an apparent viscosity is introduced instead of the dynamic viscosity. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions.

With the CFD Module, you can model flows of non-Newtonian fluids using the predefined constitutive models. The following models which describe the stress-strain relationship for non-Newtonian fluids are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou and Casson–Papanastasiou.

In theory, the same equations describe both laminar and turbulent flows. In practice, however, the mesh resolution required to simulate turbulence with the Laminar Flow interface makes such an approach impractical.

There are several books where derivations of the Navier–Stokes equations and detailed explanations of concepts such as Newtonian fluids can be found. See, for example, the classical text by Batchelor (Ref. 3) and the more recent work by Panton (Ref. 4).

Many applications describe isothermal flows for which Equation 3-13 is decoupled from Equation 3-11 and Equation 3-12. Nonisothermal flow and the temperature equation are described in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 3-11 and Equation 3-12 requires $\partial/\partial\phi$ to be zero. That is, there must be no gradients in the azimuthal direction. A common additional assumption is, however, that $u_\phi = 0$. In such cases, the ϕ-equation can be removed from Equation 3-12. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the ϕ-equation. The default 2D axisymmetric formulation of Equation 3-11 and Equation 3-12 therefore assumes that

$$\partial/\partial\phi = 0$$
$$u_\phi = 0$$

You can activate the **Swirl Flow** property which reduces the above assumptions to $\partial/\partial\phi = 0$ and reintroduces the ϕ-equation into Equation 3-12.

Compressible Flow

The equations of motion for a single-phase fluid are the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-16}$$

and the momentum equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) + \mathbf{F} \tag{3-17}$$

These equations are applicable for incompressible as well as for compressible flow with density and viscosity variations.

Weakly Compressible Flow

The same equations as for Compressible Flow are applied for weakly compressible flow. The only difference is that the density is evaluated at the reference pressure. The density may be a function of other quantities, in particular it may be temperature dependent.

The weakly compressible flow equations are valid for incompressible as well as compressible flow with density variations independent of the pressure.

Provided that the densities dependency pressure is specified through model inputs, the density is automatically evaluated at the reference pressure level.

The Mach Number Limit

An important dimensionless number in fluid dynamics is the Mach number, Ma, defined by

$$\mathrm{Ma} = \frac{|\mathbf{u}|}{a}$$

where a is the speed of sound. A flow is formally incompressible when $\mathrm{Ma} = 0$. This is theoretically achieved by letting the speed of sound tend to infinity. The Navier–Stokes equations then have the mathematical property that pressure disturbances are instantaneously propagated throughout the entire domain. This results in a parabolic equation system.

The momentum equation, Equation 3-17, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 3-16, is hyperbolic for both steady and unsteady flow. The combined system of equations is thus hybrid parabolic-hyperbolic for unsteady flow and hybrid elliptic-hyperbolic for steady flow. An exception occurs when the viscous term in Equation 3-17 becomes vanishingly small, such as at an outflow boundary, in which case the momentum equation becomes locally hyperbolic. The number of boundary conditions to apply on the boundary then depends on the number of characteristics propagating into the computational domain. For the purely hyperbolic system, the number of characteristics propagating from the boundary into the domain changes as the Mach number passes through unity. Hence, the number of boundary conditions required to obtain a numerically well-posed

system must also change. The compressible formulation of the laminar and turbulent interfaces uses the same boundary conditions as the incompressible formulation, which implies that the compressible interfaces are not suitable for flows with a Mach number larger than or equal to one. Yet, the practical Mach number limit is lower than one. The main reason is that the numerical scheme (stabilization and boundary conditions) of the Laminar Flow interface does not recognize the direction and speed of pressure waves. The fully compressible Navier–Stokes equations do, for example, start to display very sharp gradients already at moderate Mach numbers. But the stabilization for the single-phase flow interface does not necessarily capture these gradients. It is impossible to give an exact limit where the low Mach number regime ends and the moderate Mach number regime begins, but a rule of thumb is that the Mach number effects start to appear at $\mathrm{Ma} = 0.3$. For this reason, the compressible formulation is referred to as *Compressible flow (Ma<0.3)* in COMSOL Multiphysics. To model high Mach number flows, use one of The High Mach Number Flow Interfaces.

Incompressible Flow

When the temperature variations in the flow are small, a single-phase fluid can often be assumed incompressible; that is, ρ is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant ρ, Equation 3-16 reduces to

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{3-18}$$

and Equation 3-17 becomes

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} \tag{3-19}$$

Provided that the densities dependency on temperature and pressure is specified through model inputs, the density is evaluated at the reference pressure level and at the reference temperature. However, if the density is a function of other quantities such as a concentration field, or if the density is specified by a user defined expression, the user has to make sure that the density is defined as constant when the incompressible flow formulation is used.

The Reynolds Number

A fundamental characteristic in analyses of fluid flow is the Reynolds number:

$$\mathrm{Re} = \frac{\rho U L}{\mu}$$

where U denotes a velocity scale, and L denotes a representative length. The Reynolds number represents the ratio between inertial and viscous forces. At low Reynolds numbers, viscous forces dominate and tend to damp out all disturbances, which leads to laminar flow. At high Reynolds numbers, the damping in the system is very low, giving small disturbances the possibility to grow by nonlinear interactions. If the Reynolds number is high enough, the flow field eventually ends up in a chaotic state called turbulence.

Note that the Reynolds number can have different meanings depending on the length scale and velocity scale. To be able to compare two Reynolds numbers, they must be based on equivalent length and velocity scales.

The Fluid Flow interfaces automatically calculate the local cell Reynolds number $\mathrm{Re}^c = \rho|\mathbf{u}|h/(2\mu)$ using the element length h for L and the magnitude of the velocity vector u for the velocity scale U. This Reynolds number is not related to the character of the flow field, but to the stability of the numerical discretization. The risk for numerical oscillations in the solution increases as Re^c grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as: `spf.cellRe`).

Non-Newtonian Flow

For an inelastic non-Newtonian fluid, the relationship between stress and strain rate is nonlinear, and we may express the constitutive relation in terms of an apparent viscosity. For the incompressible flow, it is:

$$\mathbf{K} = 2\mu_{\mathrm{app}}(\dot{\gamma})\,\mathbf{S}$$

where $\dot{\gamma}$ is the shear rate,

$$\dot{\gamma} = \sqrt{2\mathbf{S}:\mathbf{S}}$$

and the contraction operator ":" is defined by

$$\mathbf{a}:\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm}$$

The Laminar Flow interfaces provide various predefined inelastic non-Newtonian constitutive models including Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou and Casson–Papanastasiou.

POWER LAW

The Power law model is an example of a generalized Newtonian model. It prescribes

$$\mu_{app} = m\left(\frac{\dot{\gamma}}{\dot{\gamma}_{ref}}\right)^{n-1} \tag{3-20}$$

where m, n are scalars that can be set to arbitrary values and $\dot{\gamma}_{ref}$ denotes a reference shear rate for which the default value is 1 s^{-1}. For $n > 1$, the power law describes a shear thickening (dilatant) fluid. For $n < 1$, it describes a shear thinning (pseudoplastic) fluid. A value of n equal to one gives the expression for a *Newtonian fluid*.

Equation 3-20 predicts an infinite viscosity at zero shear rate for $n < 1$. This is however never the case physically. Instead, most fluids have a constant viscosity for shear rates smaller than 10^{-2} s^{-1} (Ref. 21). Since infinite viscosity also makes models using Equation 3-20 difficult to solve, COMSOL Multiphysics implements the Power law model as

$$\mu_{app} = m\left(\frac{\max(\dot{\gamma}, \dot{\gamma}_{min})}{\dot{\gamma}_{ref}}\right)^{n-1} \tag{3-21}$$

where $\dot{\gamma}_{min}$ is a lower limit for the evaluation of the shear rate magnitude. The default value for $\dot{\gamma}_{min}$ is 10^{-2} s^{-1}, but can be given an arbitrary value or expression using the corresponding text field.

CARREAU MODEL

The Carreau model defines the viscosity in terms of the following four-parameter expression

$$\mu_{app} = \mu_\infty + (\mu_0 - \mu_\infty)[1 + (\lambda\dot{\gamma})^2]^{\frac{n-1}{2}} \tag{3-22}$$

where λ is a parameter with the unit of time, μ_0 is the zero shear rate viscosity, μ_∞ is the infinite shear-rate viscosity, and n is a dimensionless parameter. This expression is able to describe the viscosity for most stationary polymer flows.

BINGHAM–PAPANASTASIOU

Viscoplastic fluid behavior is characterized by existence of the yield stress τ_y — a limit which must be exceeded before significant deformation can occur. To model the stress-deformation behavior of viscoplastic materials, different constitutive equations have been propose. The Bingham plastic model is written as

$$\mu_{app} = \mu_p + \frac{\tau_y}{\dot{\gamma}}, \quad |\mathbf{K}| > \tau_y$$

where μ_p is the plastic viscosity.

To allow computation in both yielded and unyielded region, the Papanastasiou continuous regularization for the viscosity function is used:

$$\mu_{app} = \mu_p + \frac{\tau_y}{\dot{\gamma}}[1 - \exp(-m_p\dot{\gamma})] \tag{3-23}$$

where m_p is a scale that controls the exponential growth of stress.

HERSCHEL–BULKLEY–PAPANASTASIOU

The Herschel–Bulkley –Papanastasiou model combines the effects of the Power law the Papanastasiou continuous regularization:

$$\mu_{app} = m\left(\frac{\dot{\gamma}}{\dot{\gamma}_{ref}}\right)^{n-1} + \frac{\tau_y}{\dot{\gamma}}[1 - \exp(-m_p\dot{\gamma})] \tag{3-24}$$

where m, n are scalars that can be set to arbitrary values, and $\dot{\gamma}_{ref}$ is the reference shear rate. In case n equals one, the Bingham–Papanastasiou model is recovered. This equation is valid in both yielded and unyielded regions. The exponent m_p controls the smoothness of the viscosity function.

CASSON–PAPANASTASIOU

The Casson–Papanastasiou model combines Casson equation with the Papanastasiou regularization:

$$\mu_{app} = \left(\sqrt{\mu_p} + \sqrt{\frac{\tau_y}{\dot{\gamma}}}[1 - \exp(-\sqrt{m_p\dot{\gamma}})]\right)^2 \tag{3-25}$$

The equation is valid in both yielded and unyielded regions.

DEFINITION

The gravity force is defined from the acceleration of gravity vector, $\mathbf{g}$, and the density, ρ. Under usual conditions and in Cartesian coordinates with the z-axis in the vertical direction,

$$\mathbf{g} = \begin{pmatrix} 0 \\ 0 \\ -g_{\text{const}} \end{pmatrix}.$$

When gravity is considered, a volume force equal to $\rho\mathbf{g}$ is included in the momentum equation. For example, for laminar weakly compressible flow, it reads:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \mathbf{F} + \rho\mathbf{g} \qquad (3\text{-}26)$$

Introducing a constant reference density ρ_{ref}, and assuming that $\mathbf{g}$ is homogeneous, this equation is equivalently written:

$$\begin{aligned}&\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \\ &\nabla\cdot\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I} + \rho_{\text{ref}}\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_{\text{ref}})\right) + \mathbf{F} + (\rho-\rho_{\text{ref}})\mathbf{g}\end{aligned} \qquad (3\text{-}27)$$

where $\mathbf{r}$ is the position vector and $\mathbf{r}_{\text{ref}}$ is an arbitrary reference position vector.

From this equation, it is convenient to define the reduced pressure which accounts for the hydrostatic pressure, $\tilde{p} = p - \rho_{\text{ref}}\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_{\text{ref}})$

$$\begin{aligned}&\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot\left(-\tilde{p}\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \\ &\mathbf{F} + (\rho-\rho_{\text{ref}})\mathbf{g}\end{aligned} \qquad (3\text{-}28)$$

In Equation 3-28, the gravity force is written $(\rho-\rho_{\text{ref}})\mathbf{g}$.

INCOMPRESSIBLE FLOW

For incompressible flow the fluid density is assumed to be constant. Hence it is natural to define the reference density, ρ_{ref}, such that $\rho = \rho_{\text{ref}} = \rho(T_{\text{ref}}, p_{\text{ref}})$ which makes it possible to simplify Equation 3-28:

$$\rho_{\text{ref}}\frac{\partial \mathbf{u}}{\partial t} + \rho_{\text{ref}}\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot(-\tilde{p}\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) + \mathbf{F}$$

In some cases, even when the flow is modeled as incompressible, buoyancy should be accounted for. Using the approximation of the gravity force based on the thermal expansion coefficient (which is relevant in this case: since the density changes are small, the first order approximation is reasonably accurate), it is possible to rewrite the momentum equation with constant density and a buoyancy force:

$$\rho_{\text{ref}}\frac{\partial \mathbf{u}}{\partial t} + \rho_{\text{ref}}\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot(-\tilde{p}\mathbf{I} + \mu_{\text{ref}}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) + \mathbf{F}$$
$$-\rho_{\text{ref}}\alpha_p(T_{\text{ref}})(T - T_{\text{ref}})\mathbf{g}$$

WEAKLY COMPRESSIBLE FLOW

For weakly compressible flow the assumption is that the density depends only on the temperature. In particular, the pressure dependency of the density is neglected, and the density is evaluated at the reference pressure: $\rho = \rho(T, p_{\text{ref}})$. With the relative pressure as dependent variable, Equation 3-26 is used

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \mathbf{F} + \rho\mathbf{g}$$

With the reduced pressure as dependent variable, Equation 3-28 is used:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot\left(-\tilde{p}\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \mathbf{F} + (\rho - \rho_{\text{ref}})\mathbf{g}$$

COMPRESSIBLE FLOW

For compressible flow the density may depend on any other variable, in particular on the temperature and the pressure. Similar equations are used as for the Weakly Compressible Flow case except that the density is not evaluated at the reference pressure.

NONISOTHERMAL FLOW COUPLING

For consistency, when the **Nonisothermal Flow** coupling is active, the assumptions made for the single phase flow interface are also made in the heat transfer interface:

- Incompressible flow: the Boussinesq approximation implies that the thermal conductivity and heat capacity are also constant.

- Weakly Compressible flow: the density is evaluated at p_{ref} in the heat interface too.
- Compressible flow: no change.

PRESSURE FORMULATION

When the relative pressure is used (default option) the interface dependent variable represents the relative pressure and the absolute pressure is defined as $p_A = p_{\text{ref}} + p$. When the pressure is used to define a boundary condition (for example, when p_0 defines the pressure condition at an outlet), it represents the relative pressure. Hence defining the outlet pressure as $p_{\text{hydro,approx}} = -\rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}})$ compensates for the gravity force for an ambient reference pressure of 0 Pa when the density is constant, there is no external force, and provided p_{ref}, $\mathbf{g}$, and $\mathbf{r}_0$ are defined consistently.

When the reduced pressure is used, the interface dependent variable (named p by default) represents the reduced pressure. The absolute pressure is then defined as $p_A = p_{\text{ref}} - \rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) + p$. In this case when the pressure is used to define a boundary condition (for example, to define a pressure condition at an outlet), its value corresponds to the reduced pressure. Hence, the prescribed pressure compensates for an approximate hydrostatic pressure, $p_{\text{hydro,approx}} = -\rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}})$, which is exact only when the density is constant and there is no external force.

PRESSURE BOUNDARY CONDITION

For an immobile fluid the momentum equation simplifies to $\nabla \cdot (p\mathbf{I}) = \mathbf{F} + \rho\mathbf{g}$ or

$\nabla \cdot (-\tilde{p}\mathbf{I}) = \mathbf{F} + (\rho - \rho_{\text{ref}})\mathbf{g}$ depending on the pressure formulation.

For incompressible flow, assuming there are no external forces, this leads respectively to $p = -\rho_{\text{ref}}\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) + p_0$ or $\tilde{p} = p_0$.

For weakly compressible flow and compressible flow, since the density varies, there is no corresponding explicit expression. We have

$$p = \int_{\mathbf{r}_{\text{ref}}}^{\mathbf{r}} \rho\mathbf{g} \cdot \mathbf{dr} + p_0 \text{ and } \tilde{p} = \int_{\mathbf{r}_{\text{ref}}}^{\mathbf{r}} (\rho - \rho_{\text{ref}})\mathbf{g} \cdot \mathbf{dr} + p_0 .$$

In practice, these integrals can be problematic to evaluate. Hence, whenever possible, it is recommended to locate the pressure boundary in a region where the approximate definition of the hydrostatic pressure is applicable, or to define a boundary that is perpendicular to the gravity vector.

If it is not possible and if the pressure conditions cannot be determined, you can use a no viscous stress condition (available in the Open Boundary feature).

See Wall for the node settings.

SLIP

The Slip condition assumes that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this is a reasonable approximation if the important effect of the wall is to prevent fluid from leaving the domain. Mathematically, the constraint can be formulated as:

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}))\mathbf{n} = \mathbf{0}$$

The no-penetration term takes precedence over the Neumann part of the condition and the above expression is therefore equivalent to

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{K}_{\mathrm{n}} - (\mathbf{K}_{\mathrm{n}} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$
$$\mathbf{K}_{\mathrm{n}} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}})\mathbf{n}$$

expressing that there is no flow across the boundary and no viscous stress in the tangential direction.

For a moving wall with translational velocity $\mathbf{u}_{\mathrm{tr}}$, $\mathbf{u}$ in the above equations is replaced by the relative velocity $\mathbf{u}_{\mathrm{rel}} = \mathbf{u} - \mathbf{u}_{\mathrm{tr}}$.

For turbulent flow, turbulence variables are in general subject to homogeneous Neumann conditions. For example

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla \varepsilon \cdot \mathbf{n} = 0$$

for the k-ε model.

POROUS SLIP

The **Porous slip** option, which can be chosen in the **Porous treatment of no slip condition** list when **Enable porous media domains** is activated, results in a special treatment of **Wall** boundaries and **Interior Wall** boundaries adjacent to porous domains (**Porous Medium** feature). Namely, similar to the **Navier slip** boundary condition, no penetration and tangential stress conditions are applied at the wall:

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{K}_{\mathrm{n}} - (\mathbf{K}_{\mathrm{n}} \cdot \mathbf{n})\mathbf{n} = -\frac{\mu}{\varepsilon_{\mathrm{p}}} \frac{\mathbf{u}_{\mathrm{slip}}}{y_{\mathrm{ps}}},$$
$$\mathbf{u}_{\mathrm{slip}} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n}, \qquad \mathbf{K}_{\mathrm{n}} = \frac{\mu}{\varepsilon_{\mathrm{p}}} (\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}})\mathbf{n}$$

Here, $\mathbf{K}_n$ is the viscous wall traction, $\mathbf{n}$ is the wall normal, $\mathbf{u}_{slip}$ is the tangential velocity at the wall while real no slip is assumed to be applied at a distance d_w (half-height of the first cell adjacent to the wall) outside the wall, and is the porous slip length. An analytical derivation of the velocity profile in the boundary layer where the pressure gradient is balanced by the sum of the Darcy term, the Forchheimer drag, and the viscous term (neglecting convective terms) leads to the following expression for y_{ps}:

$$y_{ps} = \tilde{l}\left(\frac{1+X_p e^{-\xi_p}}{1-X_p e^{-\xi_p}}\right)\left[\left(\frac{1+X_p e^{-\xi_p}}{1+X_p}\right)^2 e^{\xi_p}-1\right], \quad \xi_p = \frac{d_w}{\tilde{l}}, \quad \tilde{l} = \frac{l_{pore}}{\sqrt{1+2c_\beta}},$$

$$X_p = \frac{\sqrt{1+2c_\beta}-\sqrt{1+\frac{4}{3}c_\beta}}{\sqrt{1+2c_\beta}+\sqrt{1+\frac{4}{3}c_\beta}}, \qquad c_\beta = \frac{\sqrt{1+4c_D}-1}{2}, c_D = \frac{\beta_{ND}}{\mu}\frac{\kappa^2}{\mu}|\nabla p - \rho \mathbf{g}|$$

where $l_{pore} = \sqrt{\kappa/\varepsilon_p}$ is the porous length scale, $\beta_{ND} = \rho c_F/\sqrt{\kappa}$ is the non-Darcian coefficient (c_F is the Forchheimer coefficient), $\mathbf{g}$ is the gravity vector, and ξ_p, l, X_p, c_β, c_D, are intermediate variables. This formula is used when the **Pressure-gradient formulation** is chosen and it uses the pressure gradient at the wall. By default, the **Velocity formulation** is activated and the corresponding formula is:

$$y_{ps} = \tilde{l}\,(e^{\xi_p}-1), \quad \xi_p = \frac{d_w}{\tilde{l}}, \quad \tilde{l} = \frac{l_{pore}}{\sqrt{1+2c_\beta}},$$

$$c_\beta = \left[\left(\frac{\beta_{ND}\kappa|\mathbf{u}_{slip}|}{\mu}\frac{l_{pore}}{d_w}\right)^2/2\right]^{1/3}$$

Although this formulation is an approximation, since it uses the slip velocity at the wall to reconstruct the pressure gradient, it is rather accurate. Moreover, the influence of the convective terms is partially accounted for in this formulation.

SLIDING WALL

The sliding wall option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

- In 2D, the tangential direction is unambiguously defined by the direction of the boundary, but the situation becomes more complicated in 3D. For this reason, this boundary condition has slightly different definitions in the different space dimensions.

- For 2D and 2D axisymmetric components, the velocity is given as a scalar U_w and the condition prescribes

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{u} \cdot \mathbf{t} = U_w$$

  where $\mathbf{t} = (n_y, -n_x)$ for 2D and $\mathbf{t} = (n_z, -n_r)$ for axial symmetry.
- For 3D components, the velocity is set equal to a given vector $\mathbf{u}_w$ projected onto the boundary plane:

$$\mathbf{u} = \frac{\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w)\mathbf{n}}{\left\|\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w)\mathbf{n}\right\|}\left\|\mathbf{u}_w\right\|$$

  The normalization makes $\mathbf{u}$ have the same magnitude as $\mathbf{u}_w$ even if $\mathbf{u}_w$ is not exactly parallel to the wall.

SLIP VELOCITY

In the microscale range, the flow at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a slip velocity at the boundary. Two phenomena account for this velocity: violation of the continuum hypothesis for the viscosity and flow induced by a thermal gradient along the boundary.

The following equation relates the viscosity-induced jump in tangential velocity to the tangential shear stress along the boundary:

$$\Delta u = \frac{1}{\beta}\tau_{n,t}$$

For gaseous fluids, the coefficient β is given by

$$\beta = \frac{\mu}{\left(\frac{2-\alpha_v}{\alpha_v}\right)\lambda}$$

where μ is the fluid's dynamic viscosity (SI unit: Pa·s), α_v represents the tangential momentum accommodation coefficient (TMAC) (dimensionless), and λ is the molecules' mean free path (SI unit: m). The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 17.

A simpler expression for β is

$$\beta = \frac{\mu}{L_s}$$

where L_s, the slip length (SI unit: m), is a straight channel measure of the distance from the boundary to the virtual point outside the flow domain where the flow profile extrapolates to zero. This equation holds for both liquids and gases.

Thermal creep results from a temperature gradient along the boundary. The following equation relates the thermally-induced jump in tangential velocity to the tangential gradient of the natural logarithm of the temperature along the boundary:

$$\Delta u = \sigma_T \frac{\mu}{\rho} \nabla_t \log T$$

where σ_T is the thermal slip coefficient (dimensionless) and ρ is the density of the fluid. The thermal slip coefficients range between 0.3 and 1.0 and can be found in Ref. 17.

Combining the previous relationships results in the following equation:

$$\mathbf{u} - \mathbf{u}_{w,t} = \frac{L_s}{\mu} \tau_{n,t} + \sigma_T \frac{\mu}{\rho T} \nabla_t T$$

Relate the tangential shear stress to the viscous boundary force by

$$\tau_{n,t} = \mathbf{K}_n - (\mathbf{n} \cdot \mathbf{K}_n)\mathbf{n}$$

where the components of $\mathbf{K}$ are the Lagrange multipliers that are used to implement the boundary condition. Similarly, the tangential temperature gradient results from the difference of the gradient and its normal projection:

$$\nabla_t T = \nabla T - (\mathbf{n} \cdot \nabla T)\mathbf{n}$$

Use Viscous Slip

When viscous slip is used, select Maxwell's model to calculate L_s using:

$$L_s = \left(\frac{2 - \alpha_v}{\alpha_v}\right)\lambda$$

Also see Wall for the node settings.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{wall} = 0$, and adds a tangential stress

$$\mathbf{K}_{nt} = -\frac{\mu}{\beta}\mathbf{u}_{slip}$$

where $\mathbf{K}_{nt} = \mathbf{K}_n - (\mathbf{K}_n \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$, $\mathbf{K}_n = \mathbf{K}\mathbf{n}_{wall}$, and $\mathbf{K}$ is the viscous stress tensor. β is a slip length, and $\mathbf{u}_{slip} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ is the velocity tangential to the wall. The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance β outside the wall.

The **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input.

In cases where the wall movement is nonzero, **Account for the translational wall velocity in the friction force** may be selected to use $\mathbf{u} - \mathbf{u}_{bnd} - ((\mathbf{u} - \mathbf{u}_{bnd}) \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ instead of $\mathbf{u}_{slip}$ in the friction force. Then, the extrapolated tangential velocity component is $\mathbf{u}_{bnd}$ at a distance β outside of the wall. Note that the **Velocity of sliding wall** $\mathbf{u}_w$ is always accounted for in the friction force.

The Navier Slip boundary condition is suitable for walls adjacent to a fluid-fluid interface or a free surface when solving for laminar flow. Applying this boundary condition, the contact line (fluid-fluid-solid interface) is free to move along the wall. Note that in problems with contact lines, the tangential velocity of the wall typically represents the movement of the contact line but the physical wall is not moving. In such cases, **Account for the translational wall velocity in the friction force** should not be checked.

The Navier Slip option is not available when selecting a turbulence model. For turbulent flow, a Wall feature using wall functions or automatic wall treatment is required for the contact line to be free to move along the wall.

CONSTRAINT SETTINGS

The wall feature uses three different techniques to constrain the velocity field:

- **Pointwise constraints** is the standard technique to enforce strong constraints in the finite element method. The desired value of the velocity is prescribed at each node point in the mesh. Since the constraint is enforced locally at each node, only local values are affected by the constraint and the constraints are independent of each other. The solvers can therefore eliminate both the constrained degrees of freedom and the constraint force terms, effectively reducing the number of degrees of freedom being solved for.

  The main advantage of pointwise constraints is that they enforce the constraint exactly pointwise. This means that they do not introduce any leakage of the velocity across the wall, unless specified. The main disadvantage of pointwise constraints is

that they introduce locking effects when trying to impose a no-penetration condition for the velocity, $\mathbf{u} \cdot \mathbf{n} = 0$, on curved walls or walls with sharp corners.

- **Weak constraints** is an alternative method to prescribe the velocity. It consists on enforcing the boundary condition for the velocity via *Lagrange multipliers*. Their main advantage is that the Lagrange multiplier can provide an accurate representation of the reaction flux at the wall. Their main disadvantage is that they introduce extra unknowns, and are usually difficult to combine with other constraint methods on adjacent boundaries. Moreover, they may require extra constraints for the Lagrange multipliers. For more information, see Weak Constraints in the *COMSOL Multiphysics Reference Manual*.
- **Nitsche constraints** use a numerical flux to prescribe the velocity at the wall. They impose the constraint in an integral sense rather than pointwise, and do not suffer from the locking effects introduced by pointwise constraints when trying to prescribe a no penetration condition for the velocity. They are also better behaved when prescribing nonlinear constraints. Their main disadvantage is that the constraint is only imposed approximately, and may produce small leaks. For more information, see Nitsche Constraints.

The following combination of Constraint techniques can be selected in the **Constraint Setting** sections of Wall boundary conditions:

- **Automatic** (default) use different constraint methods depending on whether only the normal component of the velocity is prescribed, such as in the no penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, imposed, for example, in Slip walls or No Slip walls using Wall Functions or Automatic Wall Treatment, or both tangential and normal components are prescribed, as is the case of No Slip walls in laminar flow.

  Nitsche constraints are used to impose the no penetration condition for Slip walls. When a No Slip condition is prescribed, pointwise constraints are used except for moving walls where Nitsche constraints are used.
- **Pointwise constraints**
- **Nitsche constraints**
- **Weak constraints** — these are not available on Interior Walls.
- **Mixed constraints** — this option is only available when both the tangential and normal components of the velocity need to be prescribed. The velocity on the wall normal direction is imposed via pointwise constraints. The constraint for the tangential directions is relaxed, and Nitsche constraints are used instead. This provides improved accuracy and performance when working with coarse boundary layer meshes. For more information, see Ref. 22.

Prescribing Inlet and Outlet Conditions

The Navier–Stokes equations can show large variations in mathematical behavior, ranging from almost completely elliptic to almost completely hyperbolic. This has implications when it comes to prescribing admissible boundary conditions. There is also a discrepancy between mathematically valid boundary conditions and practically useful boundary conditions. See Inlet and Outlet for the node settings.

INLET CONDITIONS

An inlet requires specification of the velocity components. The most robust way to do this is to prescribe a velocity field using a Velocity condition.

A common alternative to prescribing the complete velocity field is to prescribe a pressure and all but one velocity component. The pressure cannot be specified pointwise because this is mathematically over-constraining. Instead the pressure can be specified via a stress condition:

$$-p + 2\mu\frac{\partial u_n}{\partial n} = F_n \tag{3-29}$$

where $\partial u_n/\partial n$ is the normal derivative of the normal velocity component. Equation 3-29 is prescribed by the Pressure condition in the Inlet and Outlet features and the Normal stress condition in the Open Boundary and Boundary Stress features. Equation 3-29 is mathematically more stringent compared to specifying the pressure pointwise and at the same time cannot guarantee that p obtains the desired value. In practice, p is close to F_n, except for low Reynolds number flows where viscous effects are the only effects that balance the pressure. In addition to Equation 3-29, all but one velocity component must be specified. For low Reynolds numbers, this can be specified by a vanishing tangential stress condition:

$$\mu\frac{\partial u_t}{\partial n} = 0$$

which is what the Normal stress condition does. Vanishing tangential stress becomes a less well-posed inlet condition as the Reynolds number increases. The Pressure condition in the Inlet feature therefore requires a flow direction to be prescribed, which provides a well-posed condition independent of Reynolds number.

OUTLET CONDITIONS

The most common approach is to prescribe a pressure via a normal stress condition on the outlet. This is often accompanied by a vanishing tangential stress condition:

$$\mu \frac{\partial u_t}{\partial n} = 0$$

where $\partial u_t/\partial n$ is the normal derivative of the tangential velocity field. It is also possible to prescribe u_t to be zero. The latter option should be used with care since it can have a significant effect on the upstream solution.

The elliptic character of the Navier–Stokes equations mathematically permits specifying a complete velocity field at an outlet. This can, however, be difficult to apply in practice. The reason being that it is hard to prescribe the outlet velocity so that it is consistent with the interior solution at each point. The adjustment to the specified velocity then occurs across an outlet boundary layer. The thickness of this boundary layer depends on the Reynolds number; the higher the Reynolds number, the thinner the boundary layer.

ALTERNATIVE FORMULATIONS

COMSOL Multiphysics provides several specialized boundary conditions that either provide detailed control over the flow at the boundary or that simulate specific devices. In practice they often prescribe a velocity or a pressure but calculate the prescribed values using, for example, ODEs.

Normal Stress Boundary Condition

Mass Flow

The **Mass flow** boundary condition constrains the mass flowing into the domain across an inlet or outlet boundary. The mass flow can be specified in a number of ways.

POINTWISE MASS FLUX

The pointwise mass flux sets the velocity at the boundary to

$$\mathbf{u} = -\frac{m_f}{\rho}\mathbf{n}$$

where m_f is the normal mass flux and ρ is the density.

MASS FLOW RATE

The mass flow rate boundary condition sets the total mass flow through the inlet boundary according to

$$-\int_{\partial\Omega} d_{bc}\rho(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = m$$

where d_{bc} (only present in the 2D Cartesian axis system) is the boundary thickness normal to the fluid-flow domain and m is the total mass flow rate. For the outlet boundary, the mass flow rate boundary condition sets the total mass flow as

$$\int_{\partial\Omega} d_{bc}\rho(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = m$$

In addition to the constraint on the total flow across the boundary, the tangential velocity components are set to zero on the boundary

$$\mathbf{u}\times\mathbf{n} = \mathbf{0} \tag{3-30}$$

STANDARD FLOW RATE

The standard flow rate boundary condition specifies the mass flow as a standard volumetric flow rate. The mass flow through the inlet boundary is set by the equation

$$-\int_{\partial\Omega} d_{\mathrm{bc}}\frac{\rho}{\rho_{\mathrm{st}}}(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = Q_{\mathrm{sv}}$$

where d_{bc} (only present in the 2D component Cartesian axis system) is the boundary thickness normal to the fluid-flow domain, ρ_{st} is the standard density, and Q_{sv} is the standard flow rate. The standard density is defined by one of the following equations:

$$\rho_{\mathrm{st}} = \frac{M_n}{V_n}$$

$$\rho_{\mathrm{st}} = \frac{p_{\mathrm{st}}M_n}{RT_{\mathrm{st}}}$$

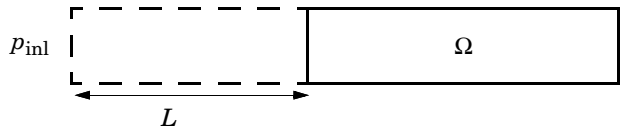
where M_n is the mean molar mass of the fluid, V_n is the standard molar volume, p_{st} is the standard pressure, R is the universal molar gas constant, and T_{st} is the standard temperature. For the outlet boundary, the mass flow rate is set by the equation

$$\int_{\partial\Omega} d_{bc}\frac{\rho}{\rho_{st}}(\mathbf{u}\cdot\mathbf{n})dS = Q_{sv}$$

Equation 3-30 or Equation 3-31 is also enforced for compressible and incompressible flow, respectively, ensuring that the normal component of the viscous stress and the tangential component of the velocity are zero at the boundary.

Fully Developed Flow (Inlet)

The **Fully developed flow** boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{inl} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$$\mathbf{u} - (\mathbf{u}\cdot\mathbf{n})\mathbf{n} = \mathbf{0}$$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$\int_{\partial\Omega}\left(\left(L\left(-\mu(\nabla_{\mathbf{t}}\mathbf{u}+(\nabla_{\mathbf{t}}\mathbf{u})^T)+\frac{(p+P_{inl})}{2}\mathbf{I}\right):(\nabla_{\mathbf{t}}\hat{\mathbf{u}})\right)-P_{inl}(\mathbf{n}\cdot\hat{\mathbf{u}})\right)$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the inlet can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω. This is

most notably if the flow is strongly curved just downstream of the inlet. This can, for example, be the case if an object is positioned just downstream of the inlet or if the adjacent boundaries are not orthogonal to the inlet. The analytical solution can in these cases be recovered by including a little bit of the inlet channel in the computational domain.

The inlet pressure, P_{inl}, must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{inl}. When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{\text{av}})\hat{P}_{\text{inl}}$$

where <·> denotes the average over the inlet. Since the equation for P_{inl} is a DAE (the equation for P_{inl} does not contain P_{inl}), it must be solved coupled to Navier–Stokes and it must be treated by a Vanka presmoother and postsmoother if iterative solvers are used.

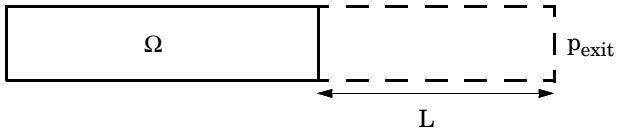
The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the inlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries). So in the figure above, if the lower boundary of Ω is a no-slip wall and the top boundary is a symmetry boundary, the lower boundary of the virtually extruded channel becomes a no-slip wall and the upper boundary becomes a symmetry boundary.

Algebraic turbulence models need additional equations or constraints. For all other turbulence models, their weak equations in the virtual inlet channel are projected onto the inlet of the computational domain. The projections are regularized to prevent the production to fall to zero, so the solutions of the projects can show slight deviation from the correct solutions close to no-slip walls.

For the Viscoelastic Flow interface, the equations for the elastic stress tensor components in the virtual inlet channel are projected onto the inlet of the computational domain.

Fully Developed Flow (Outlet)

The **Fully developed flow** boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{exit} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$\int_{\partial\Omega} \left(\left(L\left(-\mu(\nabla_{\mathbf{t}}\mathbf{u} + (\nabla_{\mathbf{t}}\mathbf{u})^T) + \frac{(p + P_{\text{exit}})}{2}\mathbf{I} \right) : (\nabla_{\mathbf{t}}\hat{\mathbf{u}}) \right) - P_{\text{exit}}(\mathbf{n} \cdot \hat{\mathbf{u}}) \right)$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the outlet can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω. The inlet pressure, P_{exit}, must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{exit}. When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{\text{av}})\hat{P}_{\text{exit}}$$

where <·> denotes the average over the inlet. Since the equation for P_{ext} is a DAE, it must be solved coupled to Navier–Stokes and it must be treated by a Vanka presmoother and postsmoother if iterative solvers are used.

The boundary conditions for the virtual outlet channel are inherited from the boundaries adjacent to the outlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

No Viscous Stress

For this module, and in addition to the Pressure, No Viscous Stress boundary condition, the viscous stress condition sets the viscous stress to zero:

$$\left(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=\mathbf{0}$$

$$(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=\mathbf{0}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

The condition is not a sufficient outlet condition since it lacks information about the outlet pressure. It must hence be combined with pressure point constraints on one or several points or lines surrounding the outlet.

This boundary condition is numerically the least stable outlet condition, but can still be beneficial if the outlet pressure is nonconstant due to, for example, a nonlinear volume force.

Normal Stress Boundary Condition

The total stress on the boundary is set equal to a stress vector of magnitude f_0, oriented in the negative normal direction:

$$\left(-p\mathbf{I}+\left(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\right)\mathbf{n}=-f_0\mathbf{n}$$

$$(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-f_0\mathbf{n}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This implies that the total stress in the tangential direction is zero. This boundary condition implicitly sets a constraint on the pressure which for 2D flows is

$$p = 2\mu\frac{\partial u_n}{\partial n} + f_0 \tag{3-31}$$

If $\partial u_n/\partial n$ is small, Equation 3-31 states that $p \approx f_0$.

The Normal Stress condition is the mathematically correct version of the Pressure Conditions condition (Ref. 4), but it is numerically less stable.

Pressure Boundary Condition

For single-phase flow, a mathematically correct natural boundary condition for outlets is

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -p_0\mathbf{n} \tag{3-32}$$

$$(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n} \tag{3-33}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This is a normal stress condition together with a no-tangential-stress condition. When $\mu > 0$, Equation 3-32 or Equation 3-33 can be supplemented with a tangential velocity condition

$$\mathbf{u}\cdot\mathbf{t} = 0 \tag{3-34}$$

If so, the no-tangential-stress condition is overridden. An issue with Equation 3-32 or Equation 3-33 is that it does not strongly enforce unidirectional flow on the boundary. If the prescribed pressure on an outlet is too high, parts of the outlet can actually have inflow. This is not as much of an issue for the Navier–Stokes equations as it is an issue for scalar transport equations solved along with the Navier–Stokes equations. Hence, when applying the **Pressure** boundary condition at an outlet or inlet you can further constrain the flow. With the **Suppress backflow** option

$$\begin{gathered}\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0\mathbf{n}\\ (-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0\mathbf{n}\\ \hat{p}_0\le p_0\end{gathered}\quad , \tag{3-35}$$

the normal stress is adjusted to keep

$$\mathbf{u}\cdot\mathbf{n}\ge 0 \tag{3-36}$$

Equation 3-35 effectively means that the prescribed pressure is p_0 if $\mathbf{u}\cdot\mathbf{n}\ge 0$, but smaller at locations where $\mathbf{u}\cdot\mathbf{n}<0$. This means that Equation 3-35 does not completely prevent backflow, but the backflow is substantially reduced. Backflow is suppressed also when external forces are acting on the fluid, provided the magnitude of these forces are of the same order as the dynamic pressure at the outlet.

A pressure condition can also be applied at an inlet. In this case, either the normal stress is prescribed

$$\begin{gathered}\mathbf{n}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0\\ \mathbf{n}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0\\ \hat{p}_0\ge p_0\end{gathered} \tag{3-37}$$

together with the tangential condition in Equation 3-34, or, a general flow direction is prescribed.

$$\begin{gathered}\mathbf{r}_\mathbf{u}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0(\mathbf{r}_\mathbf{u}\cdot\mathbf{n})\\ \mathbf{r}_\mathbf{u}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0(\mathbf{r}_\mathbf{u}\cdot\mathbf{n})\\ \hat{p}_0\ge p_0\\ \mathbf{u}-(\mathbf{u}\cdot\mathbf{r}_\mathbf{u})\mathbf{r}_\mathbf{u}=\mathbf{0},\ \mathbf{r}_\mathbf{u}=\frac{\mathbf{d}_\mathbf{u}}{\|\mathbf{d}_\mathbf{u}\|}\end{gathered} \tag{3-38}$$

The “>” option is used with suppress backflow to have $\mathbf{u}\cdot\mathbf{n}\le 0$ or $\mathbf{u}\cdot\mathbf{r}_\mathbf{u}\ge 0$.

For incompressible single-phase flow, it is also allowed to specify the total pressure, p_{tot}, instead of the static pressure, p_{stat}, on inlet and outlet boundaries. It is more

useful, for example, in pump applications. The pressure is then prescribed at the boundaries using Bernoulli's principle,

$$p = p_{\text{stat}} = p_{\text{tot}} - \frac{1}{2}\rho|\mathbf{u}|^2 \tag{3-39}$$

The equation is imposed with two options: **Average** and **Pointwise**.

In the first option, p_{stat} is prescribed by:

$$\mathbf{n}^T(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = \mathbf{n}^T(-p_{\text{stat}}\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} \tag{3-40}$$

where p_{tot} and $|\mathbf{u}|^2$ are averaged over the boundaries using the `aveop` operator:

$$p_{\text{stat}} = \text{aveop}(p_{\text{tot}}) - \frac{1}{2}\rho \cdot \text{aveop}(|\mathbf{u}|^2)$$

For the second option, Equation 3-39 is prescribed pointwise.

See Inlet, Outlet, Open Boundary, and No Viscous Stress for the individual node settings. Note that some modules have additional theory sections describing options available with that module.

Vacuum Pump Boundary Condition

Vacuum pumps (devices) can be represented using lumped curves implemented as boundary conditions. These simplifications also imply some assumptions. In particular, it is assumed that a given boundary can only be an outlet. Such a boundary should not be a mix of inlets/outlets nor switch between them during a simulation.

Manufacturers usually provide curves that describe the pumping rate as a function of suction pressure for a vacuum pump. Also see Vacuum Pump for the node settings.

DEFINING A DEVICE AT AN OUTLET

In this case (see Figure 3-2), the device's inlet is the interior face situated between the blue (cube) and green (circle) domains while its outlet is an external boundary, here the circular boundary of the green domain. The lumped curve gives the pumping rate as a function of the pressure at the suction side of the vacuum pump. This boundary condition implementation follows the Fully Developed Flow (Outlet) boundary condition with the Flow Rate option:

$$\int_{\partial\Omega_{out}} \mathbf{u} \cdot \mathbf{n} dS = V_0 \tag{3-41}$$

Here, V_0 is the pumping rate function of suction pressure for the vacuum pump. In 2D the thickness in the third direction, D_z, is used to define the flow rate. Vacuum pumps are modeled as rectangles in this case.

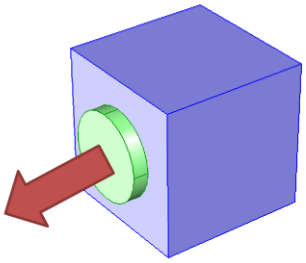


Figure 3-2: A vacuum pump at the outlet. The arrow represents the flow direction, the green circle represents the vacuum pump (that should not be part of the model), and the blue cube represents the modeled domain with an outlet boundary condition described by a lumped curve for the attached vacuum pump.

Fan Defined on an Interior Boundary

In this case, the inlet and outlet of the device are both interior boundaries (see Figure 3-3). The boundaries are called `dev_in` and `dev_out`. The boundary conditions are described as follows:

- The inlet of the device is an outlet boundary condition for the modeled domain. For this outlet side, on `dev_in`, a pressure condition is set. The value of the pressure is set to the sum of the mean value of the pressure on `dev_out` and the pressure drop across the device. The pressure drop is calculated from a lumped curve using the flow rate evaluated on `dev_in`.
- For the inlet side, on `dev_out`, a pressure boundary condition is defined. The pressure value is set so that the flow rate is equal on `dev_in` and `dev_out`. An ODE is added to compute the pressure value.
- When a turbulence model with transport equations for the turbulence quantities is applied, the turbulent kinetic energy, k, and dissipation rate, ε, or specific dissipation rate, ω, must be specified on the downstream side of the fan. When the v2-f

turbulence model is used, the turbulent relative fluctuations, ζ, must also be specified, and with the transition model in the SST turbulence model, also γ.The turbulence conditions are specific to the design and operating conditions of the fan. A reference velocity scale U_{ref} is available in order to set default values.

$$k_{0\text{init}} = 0.015U_{\text{ref}}^2, \quad \varepsilon_{0\text{init}} = \frac{C_\mu^{3/4} k_{0\text{init}}^{3/2}}{l_{\text{ref}}} \tag{3-42}$$

	In both cases, the boundary condition implementation follows the Pressure Boundary Condition for outlet or inlet with the Suppress backflow option.

	See Interior Fan for node settings.

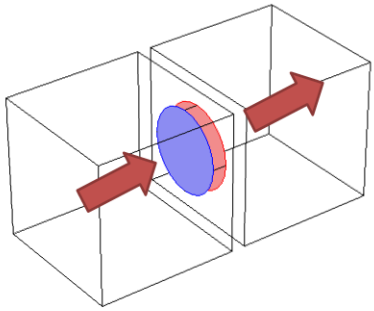


Figure 3-3: A device between two boundaries. The red arrows represent the flow direction, the cylindrical part represents the device (that should be not be part of the model), and the two cubes are the domain that are modeled with a particular inlet boundary condition to account for the device.

Fan and Grille Boundary Conditions

Fans, pumps, or grilles (devices) can be represented using lumped curves implemented as boundary conditions. These simplifications also imply some assumptions. In particular, it is assumed that a given boundary can only be either an inlet or an outlet. Such a boundary should not be a mix of inlets and outlets, nor switch between them during a simulation.

Manufacturers usually provide curves that describe the static pressure as a function of flow rate for a fan. See Fan and Grille for the node settings.

DEFINING A DEVICE AT AN INLET

In this case, the device's inlet is an external boundary, represented by the external circular boundary of the green domain on Figure 3-4. The device's outlet is an interior face situated between the green and blue domains in Figure 3-4. The lumped curve gives the flow rate as a function of the pressure difference between the external boundary and the interior face. This boundary condition implementation follows the Pressure Boundary Condition for inlets with the Suppress backflow option:

$$\mathbf{n}^{\mathrm{T}}\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0 \qquad \hat{p}_0\geq p_{\mathrm{input}}+\Delta p_{\mathrm{fan}}(V_0) \tag{3-43}$$

The Grille boundary condition sets the following conditions:

$$\mathbf{n}^{\mathrm{T}}\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0 \qquad \hat{p}_0\geq p_{\mathrm{input}}+\Delta p_{\mathrm{grille}}(V_0) \tag{3-44}$$

Here, V_0 is the flow rate across the boundary, p_{input} is the pressure at the device's inlet, and $\Delta p_{\mathrm{fan}}(V_0)$ and $\Delta p_{\mathrm{grille}}(V_0)$ are the static pressure functions of flow rate for the fan and the grille. Equation 3-43 and Equation 3-44 correspond to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla\cdot\mathbf{u})$ vanishes. When a turbulence model with a transport equation for the turbulent kinetic energy is applied, the term $-(2/3)\rho k$ appears on the left sides of Equation 3-43 and Equation 3-44. In such cases the turbulent kinetic energy, k, the turbulent relative fluctuations, ζ (for the v2-f turbulence model), and dissipation rate, ε, or specific dissipation rate, ω, must be specified on the downstream side. The turbulence conditions are specific to the design and operating conditions of the fan or grille. For the Fan condition, a reference velocity scale U_{ref} is available in order to set default values according to Equation 3-42. For the Grille boundary condition the turbulence quantities on the downstream side are specified by defining a loss coefficient $K=2\Delta p_{\mathrm{grille}}/\rho(\mathbf{u}\cdot\mathbf{n})^2$, from which a refraction coefficient is derived using Equation 3-57. Equation 3-50 through Equation 3-52 are then used to relate upstream and downstream turbulence quantities.

When an algebraic turbulence model, such as the Algebraic yPlus or L-VEL model, is used, the turbulence is only implicitly affected by the device through the change in the local Reynolds number.

The flow direction is enforced to be normal to the boundary by default. However, it is possible to define an arbitrary inflow velocity direction. In such case, Equation 3-43 and Equation 3-44 are modified similarly to Equation 3-38. In 2D, the thickness in the third direction, *Dz*, is used to define the flow rate. Fans are modeled as rectangles in this case.

For 3D and 2D axisymmetry when the swirl flow is included, it is possible to define a swirl on the downstream side of the fan. It sets the following boundary conditions:

$$\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0$$

$$\mathbf{u}\cdot\mathbf{t}=\mathbf{u}_{\mathrm{swirl}}=c_{\mathrm{sf}}2\pi f\mathbf{n}\times(\mathbf{r}-\mathbf{r}_{\mathrm{bp}})$$

$$\hat{p}_0\geq p_{\mathrm{input}}+\Delta p_{\mathrm{fan}}$$

Here, the swirl ratio c_{sf} is a positive number less than 1, defining the ratio of the rotation transferred from the fan to the flow, f is the number of revolutions per time for the fan, and $\mathbf{r}_{\mathrm{bp}}$ is the rotation axis base point. The swirl velocity is defined on the maximum inscribed circular region on the fan inlet boundary. Hence, it is only applicable on simply connected flat boundaries. For more complicated inlet topologies, a swirl velocity can be defined by specifying the inlet velocity vector.

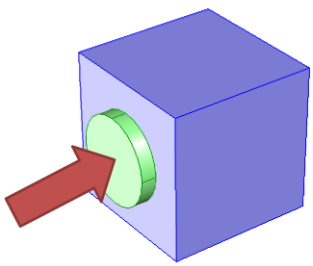


Figure 3-4: A device at the inlet. The arrow represents the flow direction, the green circle represents the device (that should not be part of the model), and the blue cube represents the modeled domain with an inlet boundary condition described by a lumped curve for the attached device.

DEFINING A DEVICE AT AN OUTLET

In this case (see Figure 3-16), the fan's inlet is the interior face situated between the blue (cube) and green (circle) domain while its outlet is an external boundary, here the circular boundary of the green domain. The lumped curve gives the flow rate as a function of the pressure difference between the interior face and the external boundary. This boundary condition implementation follows the Pressure Boundary Condition for outlets with the Suppress backflow option:

$$\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0\mathbf{n} \qquad (3\text{-}45)$$
$$\hat{p}_0\le p_{\mathrm{exit}}-\Delta p_{\mathrm{fan}}(V_0)$$

The Grille boundary condition sets the following conditions:

$$\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0\mathbf{n} \qquad (3\text{-}46)$$
$$\hat{p}_0\le p_{\mathrm{exit}}-\Delta p_{\mathrm{grille}}(V_0)$$

Here, V_0 is the flow rate across the boundary, p_{exit} is the pressure at the device outlet, and $\Delta p_{\mathrm{fan}}(V_0)$ and $\Delta p_{\mathrm{grille}}(V_0)$ are the static pressure function of flow rate for the fan and the grille. Equation 3-45 and Equation 3-46 correspond to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla\cdot\mathbf{u})\mathbf{n}$ vanishes. When a turbulence model with a transport equation for the turbulence kinetic energy is applied, the term $-(2/3)\rho k\mathbf{n}$ appears on the left sides of Equation 3-45 and Equation 3-46. In 2D the thickness in the third direction, *Dz*, is used to define the flow rate. Fans are modeled as rectangles in this case.

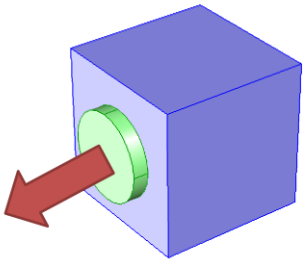


Figure 3-5: A fan at the outlet. The arrow represents the flow direction, the green circle represents the fan (that should not be part of the model), and the blue cube represents the

modeled domain with an outlet boundary condition described by a lumped curve for the attached fan.

Screen Boundary Condition

The word "screen" refers to a barrier with distributed perforations such as a wire gauze, grille, or perforated plate. The screen is assumed to have a width, which is small compared to the resolved length-scales of the flow field and can thus be modeled as an edge (in 2D) or surface (in 3D). This idea permits an economic implementation of the screen, where the details of the barrier need not be resolved. A limitation to this type of modeling may be observed when there is an appreciable velocity component parallel to the screen. In such cases the pressure may become discontinuous across streamlines, which may lead to convergence problems. If this occurs, a better approach is to model the screen as a thin domain with distributed momentum-loss terms.

The general influence of a screen on the flow field is a loss in the normal momentum component, a change in direction (related to a suppression of the tangential velocity component), attenuation of the turbulence kinetic energy and preservation of the turbulence length scale (Ref. 18). The conditions across the screen are expressed as

$$[\rho \mathbf{u} \cdot \mathbf{n}]_-^+ = 0 \tag{3-47}$$

$$\left[\rho(\mathbf{u}\cdot\mathbf{n})^2 + p - \mathbf{n}^T\left\{(\mu+\mu_T)\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T - \frac{2}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right) - \frac{2}{3}\rho k\mathbf{I}\right\}\mathbf{n}\right]_-^+ = -\frac{K}{2}\rho_-(\mathbf{u}_-\cdot\mathbf{n})^2 \tag{3-48}$$

$$\mathbf{n}\times\mathbf{u}_+ = \eta(\mathbf{n}\times\mathbf{u}_-) \tag{3-49}$$

$$k_+ = \eta^2 k_- \tag{3-50}$$

and, depending on the turbulence model in use, either

$$\varepsilon_+ = \eta^3\varepsilon_- \tag{3-51}$$

or

$$\omega_+ = \eta\omega_- \tag{3-52}$$

Here, '–' and '+' refer to the upstream and downstream side of the screen, respectively. Furthermore, K is the dimensionless resistance coefficient, which parameterizes the magnitude of the drag exerted by the screen on the flow. η is the dimensionless refraction coefficient, which parameterizes the extent to which the screen causes the flow to change direction to align parallel to the normal downstream direction from the plane of the screen. The refraction coefficient should be between 0 and 1. Isotropic turbulence is expected on the downstream side of the screen, hence,

$$\zeta_+ = \frac{2}{3} \tag{3-53}$$

is enforced when the v2-f turbulence model is used.

The attenuation of the turbulence kinetic energy (Equation 3-50) is based on the suppression of the tangential velocity (Equation 3-49) and the changes in ε and ω are determined by the assumption of preservation of the turbulence length-scale across the screen.

When the transition model is active for the SST model, continuity of intermittency, γ, is applied across the screen.

For algebraic turbulence model, such as the Algebraic yPlus or L-VEL model, the turbulence is only implicitly affected by the device through the change in the local Reynolds number.

The Screen feature provides three commonly used correlations for K (Ref. 19). The following correlation is valid for wire gauzes

$$K = (0.52 + 0.66/\mathrm{Re}_d^{4/3})((1-\sigma_s)^{-2} - 1), \mathrm{Re}_d = |\mathbf{u}|d/\nu \tag{3-54}$$

Here σ_s is the solidity (ratio of blocked area to total area of the screen) and d is the diameter of the wires. For a square mesh, the correlation

$$K = 0.98((1-\sigma_s)^{-2} - 1)^{1.09} \tag{3-55}$$

is applied whereas for a perforated plate

$$K = 0.94((1-\sigma_s)^{-2} - 1)^{1.28} \tag{3-56}$$

holds. These correlations are based on common shapes for meshes and perforated plates encountered in engineering contexts, and it is assumed that the wire gauze, square mesh or perforated plate is thin compared to the mixing length scale up- and downstream of the screen. The following correlation for wire gauzes (Ref. 20) gives

reasonable values for η for a wide range of applications and has been included in the implementation:

$$\eta = \sqrt{\frac{K^2}{16} + 1} - \frac{K}{4} \tag{3-57}$$

See Screen for the node settings. Also see Theory for the Nonisothermal Screen Boundary Condition for the nonisothermal version of these physics interfaces.

Porous Interface

This condition properly accounts for a sudden jump in porosity ε_p across boundary between different domains, giving the corresponding jump in stress across the interface. The emergence of a boundary layer on the upstream side of the interface is also revealed, which provides modifications to the behavior of the tangential velocity near the interface. The feature helps to avoid the need to add a very thin transition region, in which $\varepsilon_{p,upstream}$ changes to $\varepsilon_{p,downstream}$ continuously, while solving the Brinkman equation in such situations. Below, '–' and '+' (used as subscripts and superscripts) refer to the upstream and downstream side of the interface, respectively.

Whatever the option for **Continuity conditions** is chosen, the velocity conditions are

$$[\rho(\mathbf{u}\cdot\mathbf{n})]\Big|_{-}^{+} = 0, \qquad \mathbf{u}_t\Big|_{-}^{+} \equiv [\mathbf{u} - (\mathbf{u}\cdot\mathbf{n})\mathbf{n}]\Big|_{-}^{+} = 0$$

That is, the mass flux and tangential velocity across the interface are constant, and $\mathbf{n}$ is assumed to be a normal pointing from '–' to '+'. **Velocity and stress** option just imposes usual stress continuity adding a correction for a possible jump in density:

$$\left[p\mathbf{n} - \mathbf{K}\mathbf{n} + \rho(\mathbf{u}\cdot\mathbf{n})\left(\left[\frac{1}{\varepsilon_p}\right]_{av}\right)^2\mathbf{u}\right]\Bigg|_{-}^{+} = 0$$

The option **Velocity and porosity-corrected stress** (default) adds a contribution due to the inertial term, which is nontrivial (gives nonzero effect) when ε_p jumps across the interface:

$$\left[p\mathbf{n}-\mathbf{K}\mathbf{n}+\rho(\mathbf{u}\cdot\mathbf{n})\left(\left[\frac{1}{\varepsilon_p}\right]_{av}\right)^2\mathbf{u}+\rho(\mathbf{u}\cdot\mathbf{n})\left(\frac{1}{2\varepsilon_p^2}\right)\mathbf{u}_{av}\right]\Bigg|_-^+ = 0$$

Notice that $\left[\frac{1}{\varepsilon_p}\right]_{av} = \left(\left[\frac{1}{\varepsilon_p}\right]_- + \left[\frac{1}{\varepsilon_p}\right]_+\right)/2$, $\mathbf{u}_{av} = (\mathbf{u}_- + \mathbf{u}_+)/2$ and so on.
Then, the **Velocity and porosity-corrected stress with loss** option has a 'pressure loss' term:

$$\left[p\mathbf{n}-\mathbf{K}\mathbf{n}+\rho(\mathbf{u}\cdot\mathbf{n})\left(\left[\frac{1}{\varepsilon_p}\right]_{av}\right)^2\mathbf{u}+\rho(\mathbf{u}\cdot\mathbf{n})\left(\frac{1}{2\varepsilon_p^2}\right)\mathbf{u}_{av}\right]\Bigg|_-^+ + p^{(\mathrm{loss})}\mathbf{n} = 0$$

This loss occurs in the downstream direction. Its mechanism is similar to the mechanism of common engineering 'total pressure loss'. Indeed, 'expansion' and 'contraction' across the interface experienced by the flow on the microscopic level (due to increasing or decreasing porosity, ε_p, respectively), are roughly equivalent to expansion and contraction of flow in a pipe with geometrical variations. Accordingly, it is assumed that only the normal velocity component is responsible for the loss. In the case of normal flow and negligible viscous term the pipe-analogy is quite exact.

Subsequently, **Pressure loss model** should be specified. Choosing **User-defined loss coefficients** requires values of **Expansion loss coefficient** and **Contraction loss coefficient** ($K_{exp} = 1$ and $K_{contr} = 0.5$ are default values). The resulting losses on the 'expansion' and 'contraction' boundaries are:

$$p^{(\mathrm{loss,expansion})} = K_{\mathrm{exp}}\left(\left(\frac{\rho(\mathbf{u}\cdot\mathbf{n})^2}{2\varepsilon_p^2}\right)_-\right),$$

$$p^{(\mathrm{loss,contraction})} = K_{\mathrm{contr}}\left(\frac{\rho(\mathbf{u}\cdot\mathbf{n})^2}{2\varepsilon_p^2}\right)_+$$

Borda–Carnot option results in the following losses:

$$p^{(\mathrm{loss,expansion})} = \frac{\rho_{av}}{2}\left(\left[\frac{(\mathbf{u}\cdot\mathbf{n})}{\varepsilon_p}\right]_+ - \left[\frac{(\mathbf{u}\cdot\mathbf{n})}{\varepsilon_p}\right]_-\right)^2,$$

$$p^{(\mathrm{loss,contraction})} = \frac{1}{2}\left(\frac{\rho(\mathbf{u}\cdot\mathbf{n})^2}{\varepsilon_p^2}\right)_+\left(\frac{1}{c_{vc}}-1\right)^2$$

and requires to choose **Vena contracta model**. The **User defined** option asks for value of **Vena contracta coefficient** ($c_{\mathrm{vc}} = 0.5$ by default). **Weisbach** option computes the coefficient based on the ratio of porosities across the interface:

$$c_{\mathrm{vc}} = c_{\mathrm{vc,ll}} + (1 - c_{\mathrm{vc,ll}})\left(\frac{\varepsilon_{\mathrm{p},+}}{\varepsilon_{\mathrm{p},-}}\right)^{n_{\mathrm{vc}}}$$

and requires inputs for **Lower limit** and **Exponent** ($c_{\mathrm{vc,ll}} = 0.63$ and $n_{\mathrm{vc}} = 3$ are default values).

Although the velocity conditions formally look the same for all **Continuity conditions** options, the latter two (containing the inertial correction due to the porosity jump) lead to an extra nontrivial effect. Namely, the tangential velocity exponentially evolves over a boundary layer formed on the upstream side of the interface boundary. This boundary layer has a characteristic length equal to

$$l_{-} = \frac{\mu\varepsilon_{\mathrm{p},-}}{\rho(\mathbf{u}\cdot\mathbf{n})}$$

The ratio of the tangential velocities right after the interface ('downstream') and outside the boundary layer ('upstream infinity') is

$$\frac{\left|\mathbf{u}_{\mathrm{t},+}\right|}{\left|\mathbf{u}_{\mathrm{t,upstream\ infinity}}\right|} = \frac{2\varepsilon_{\mathrm{p},+}/\varepsilon_{\mathrm{p},-}}{\varepsilon_{\mathrm{p},+}/\varepsilon_{\mathrm{p},-} + \varepsilon_{\mathrm{p},-}/\varepsilon_{\mathrm{p},+}}$$

In terms of the interstitial velocity, $\mathbf{u}^{(i)} = \mathbf{u}/\varepsilon_{\mathrm{p}}$, this results in:

$$\frac{\left|\mathbf{u}^{(\mathrm{i})}{}_{\mathrm{t},+}\right|}{\left|\mathbf{u}^{(\mathrm{i})}{}_{\mathrm{t,upstream\ infinity}}\right|} = \frac{2}{\varepsilon_{\mathrm{p},+}/\varepsilon_{\mathrm{p},-} + \varepsilon_{\mathrm{p},-}/\varepsilon_{\mathrm{p},+}} \le 1$$

Obviously, tangential component of the interstitial kinetic energy is lost across the interface. For low viscosity and high normal-flow component, when l_u is much lower than l_{geom} (the characteristic geometry length) there are apparent variations in $\mathbf{u}_t$ and $\mathbf{u}^{(i)}{}_t$ in a thin boundary layer on the upstream side of the interface. However, for the cases with high viscosity or nearly interface-parallel flow, l_u is much larger than l_{geom}, and any variations in $\mathbf{u}_t$ and $\mathbf{u}^{(i)}{}_t$ are virtually invisible.

Notice that the feature does not take into account possible underresolved porous scale, as is described in Theory for the Free and Porous Media Flow, Darcy Interface.

Mass Sources for Fluid Flow

There are two types of mass sources in a Single-Phase Flow interface: point sources and line sources.

These features require at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, Polymer Flow Module, or Subsurface Flow Module.

POINT SOURCE

A point source is theoretically formed by taking a mass injection/ejection, $\dot{Q}$ (SI unit: kg/(m^3·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_\mathrm{p}$ (SI unit: kg/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q} = \dot{q}_\mathrm{p} \tag{3-58}$$

An alternative way to form a point source/sink is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant, results in the same point source. For this alternative approach, effects resulting from the physical object volume, such as drag and fluid displacement, need to be neglected.

The weak contribution

$$\dot{q}_\mathrm{p}\mathrm{test}(p)$$

is added to a point in the geometry. As can be seen from Equation 3-58, $\dot{Q}$ must tend to plus or minus infinity as δV tends to zero. This means that in theory the pressure also tends to plus or minus infinity.

Observe that “point” refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 3-58 corresponds to a finite pressure in a point with the effect of the point source spread out over a region around the point.

The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region, but also a more extreme pressure value. It is important not to mesh too finely around a point source since the resulting pressure can result in unphysical values for the density, for example. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}$ (SI unit: kg/(m^3·s)), located within a tube with cross-sectional area δS and then letting δS tend to zero, while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_1$ (SI unit: kg/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_1 \tag{3-59}$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects on the fluid resulting from the physical object volume are neglected.

The weak contribution

$$\dot{q}_1 \text{test}(p)$$

is added to lines in 3D or to points in 2D (which represent cut-through views of lines). Line sources can also be added to the axisymmetry line in 2D axisymmetry components. It cannot, however, be added to geometrical lines in 2D because they represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

For feature node information, see Line Mass Source and Point Mass Source in the *COMSOL Multiphysics Reference Manual*.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, these shared physics nodes are renamed as follows:

- The **Line Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).
- The **Point Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

Numerical Stability — Stabilization Techniques for Fluid Flow

The momentum equation (Equation 3-17 or Equation 3-19) is a (nonlinear) convection-diffusion equation. Such equations can easily become unstable if discretized using the Galerkin finite element method. Stabilized finite element methods are usually necessary in order to obtain physical solutions. The stabilization settings are found in the main Fluid Flow interface features. To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There are three types of stabilization methods available for Navier–Stokes — *streamline diffusion*, *crosswind diffusion*, and *isotropic diffusion*. Streamline diffusion and crosswind diffusion are consistent stabilization methods, whereas isotropic diffusion is an inconsistent stabilization method.

For optimal functionality, the exact weak formulations of and constants in the streamline diffusion and crosswind diffusion methods depend on the order of the shape functions (basis functions) for the elements. The values of constants in the streamline diffusion and crosswind diffusion methods follow Ref. 5 and Ref. 6.

STREAMLINE DIFFUSION

For strongly coupled systems of equations, the streamline diffusion method must be applied to the system as a whole rather than to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 8) and were later extended to Galerkin least-squares (GLS) applied to the Navier–Stokes equations (Ref. 9). This is the streamline diffusion formulation that COMSOL Multiphysics supports.

Streamline diffusion is active by default because it is necessary when convection is dominating the flow.

The governing equations for incompressible flow are subject to the Babuška–Brezzi condition, which states that the shape functions (basis functions) for pressure must be of lower order than the shape functions for velocity. If the incompressible Navier–Stokes equations are stabilized by streamline diffusion, it is possible to use equal-order interpolation. Hence, streamline diffusion is necessary when using first-order elements for both velocity and pressure. This applies also if the model is solved using geometric multigrid (either as a solver or as a preconditioner) and at least one multigrid hierarchy level uses linear Lagrange elements.

CROSSWIND DIFFUSION

Crosswind diffusion can also be formulated for systems of equations, and when applied to the Navier–Stokes equations it becomes a shock-capturing operator. COMSOL Multiphysics supports the formulation in Ref. 9 with a shock-capturing viscosity of the Hughes–Mallet type Ref. 8.

Incompressible flows do not contain shock waves, but crosswind diffusion is still useful for introducing extra diffusion in sharp boundary layers and shear layers that otherwise would require a very fine mesh to resolve.

Crosswind diffusion is active by default as it makes it easier to obtain a solution even if the problem is fully resolved by the mesh. Crosswind diffusion also enables the iterative solvers to use inexpensive presmoothers. If crosswind diffusion is deactivated, more expensive preconditioners must be used instead.

STABILIZATION TIME SCALES

The time-scale tensor for time-dependent problems should in theory depend on a time-scale that many references just set to the time-step taken by the time-solver, Δt (see, for example, Ref. 9 and Ref. 10). This simple approach does not, however, necessarily reflect on the actual time-scales in the physics. A typical example is reacting flows where the time step is often guided by fast reactions, while the flow develops relatively slowly. The COMSOL Multiphysics software can therefore replace Δt^2 in the time-scale tensor with measures of type $(1/(\Delta \tilde{t})^2)^{-1}$, which are calculated from projections of weak expressions in a fashion similar to those in Ref. 11. These measures of the time scale are used when **Use dynamic subgrid time scale** is activated.

The **Limit small time steps effect on stabilization time scale** option can be used to ramp down the time-step contribution in the stabilization when the time step becomes much smaller than the convective and diffusive time scales. This option prevents loss of pressure stabilization at such small time steps.

ISOTROPIC DIFFUSION

Isotropic diffusion adds diffusion to the Navier–Stokes equations. Isotropic diffusion significantly reduces the accuracy of the solution but does a very good job at reducing oscillations. The stability of the continuity equation is not improved.

Numerical Stabilization and Iterative in the *COMSOL Multiphysics Reference Manual*

Solvers for Laminar Flow

The Navier–Stokes equations constitute a nonlinear equation system. A nonlinear solver must hence be applied to solve the problem. The nonlinear solver iterates to reach the final solution. In each iteration, a linearized version of the nonlinear system is solved using a linear solver. In the time-dependent case, a time marching method must also be applied. The default suggestions for each of these solver elements are discussed below.

NONLINEAR SOLVER

The nonlinear solver method depends on if the model solves a stationary or a time-dependent problem.

Stationary Solver

In the stationary case, a fully coupled, damped Newton method is applied. The initial damping factor is low since a full Newton step can be harmful unless the initial values are close to the final solution. The nonlinear solver algorithm automatically regulates the damping factor in order to reach a converged solution.

For advanced models, the automatically damped Newton method might not be robust enough. A pseudo time-stepping algorithm can then be invoked. See Pseudo Time Stepping for Laminar Flow Models.

Time-Dependent Solver

In the time-dependent case, the initial guess for each time step is (loosely speaking) the previous time step, which is a very good initial value for the nonlinear solver. The automatic damping algorithm is then not necessary. The damping factor in the Newton method is instead set to a constant value slightly smaller than one. Also, for the same reason, it suffices to update the Jacobian once per time step.

It is seldom worth the extra computational cost to update the Jacobian more than once per time step. For most models it is more efficient to restrict the maximum time step or possibly lower the damping factor in the Newton method.

LINEAR SOLVER

The linearized Navier–Stokes equation system has saddle point character, unless the density depends on the pressure. This means that the Jacobian matrix has zeros on the diagonal. Even when the density depends on the pressure, the equation system effectively shares many numerical properties with a saddle point system.

For small 2D and 3D models, the default solver suggestion is a direct solver. Direct solvers can handle most nonsingular systems and are very robust and also very fast for small models. Unfortunately, they become slow for large models and their memory requirement scales as somewhere between $N^{1.5}$ and N^2, where N is the number of degrees of freedom in the model. The default suggestion for large 2D and 3D models is therefore the iterative GMRES solver. The memory requirement for an iterative solver optimally scales as N.

GMRES is accelerated by a multigrid method, per default the smoothed aggregation algebraic multigrid (SAAMG) method. The cost of SAAMG is typically very low compared to the number of GMRES iterations necessary if no multigrid method is used. As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, the geometric multigrid (GMG) method requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared-memory computations with many cores. When the default linear solver is GMRES, an optional, but deactivated, linear solver node is available where GMRES is accelerated by GMG.

Multigrid methods need smoothers, but the saddle point character of the linear system restricts the number of applicable smoothers. The choices are further restricted by the anisotropic meshes frequently encountered in fluid-flow problems. The efficiency of the smoothers is highly dependent on the numerical stabilization. Iterative solvers perform at their best when both Streamline Diffusion and Crosswind Diffusion are active.

The default smoother for P1+P1 elements is SCGS. This is an efficient and robust smoother specially designed to solve saddle point systems on meshes that contain anisotropic elements. The SCGS smoother works well even without crosswind diffusion. SCGS can sometimes work for higher-order elements, especially if **Method** in the SCGS settings is set to **Mesh element lines**. But there is no guarantee for this, so the

default smoother for higher order elements is an SOR Line smoother. SOR Line handles mesh anisotropy but does not formally address the saddle point character. It does, however, function in practice provided that streamline diffusion and crosswind diffusion are both active.

A different kind of saddle point character can arise if the equation system contains ODE variables. Some advanced boundary conditions, for example, Fully Developed Flow (Inlet), can add equations with such variables. These variables must be treated with the Vanka algorithm. SCGS includes an option to invoke Vanka. Models with higher-order elements must apply SCGS or use the Vanka smoother. The latter is the default suggestion for higher-order elements, but it does not work optimally for anisotropic meshes.

TIME-DEPENDENT SOLVERS

The default time-dependent solver for Navier–Stokes is the BDF method with maximum order set to two. Higher BDF orders are not stable for transport problems in general nor for Navier–Stokes in particular.

BDF methods have been used for a long time and are known for their stability. However, they can have severe damping effects, especially the lower-order methods. Hence, if robustness is not an issue, a model can benefit from using the generalized-α method instead. Generalized-α is a solver that has properties similar to those of the second-order BDF solver but it is much less diffusive.

Both BDF and generalized-α are per default set to automatically adjust the time step. While this works well for many models, extra efficiency and accuracy can often be gained by specifying a maximum time step. It is also often beneficial to specify an initial time step to make the solver progress smoothly in the beginning of the time series.

In the *COMSOL Multiphysics Reference Manual:*

- Time-Dependent Solver
- Multigrid, Direct, Iterative, SCGS, SOR Line, and Vanka
- Stationary Solver

Pseudo Time Stepping for Laminar Flow Models

A stationary formulation has per definition no time derivatives and Equation 3-19 reduces to:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F} \tag{3-60}$$

Solving Equation 3-60 requires a starting guess that is close enough to the final solution. If no such guess is at hand, the fully transient problem can be solved instead. This is, however, a rather costly approach in terms of computational time. An intermediate approach is to add a fictitious time derivative to Equation 3-60:

$$\rho\frac{\mathbf{u}-\text{nojac}(\mathbf{u})}{\tilde{\Delta t}}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F}$$

where $\tilde{\Delta t}$ is a *pseudo time step*. Since $\mathbf{u}$–nojac($\mathbf{u}$) is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a step of size $\tilde{\Delta t}$ of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step $\tilde{\Delta t}$ can be chosen individually for each element based on the local CFL number:

$$\tilde{\Delta t} = \text{CFL}_{\text{loc}}\frac{h}{|\mathbf{u}|}$$

where h is the mesh cell size. A small CFL number means a small time step. It is practical to start with a small CFL number and gradually increase it as the solution approaches steady state.

If the automatic expression for CFL_{loc} is set to the built-in variable `CFLCMP`, then the automatic setting suggests a PID regulator for the pseudo time step in the default solver. The PID regulator starts with a small CFL number and increases CFL_{loc} as the solution comes closer to convergence.

The default manual expression is

$$\begin{aligned}&1.3^{\min(\text{niterCMP},\,9)}+\\ &\text{if}(\text{niterCMP}>20,\,9\cdot 1.3^{\min(\text{niterCMP}-20,\,9)},\,0)+\\ &\text{if}(\text{niterCMP}>40,\,90\cdot 1.3^{\min(\text{niterCMP}-40,\,9)},\,0)\end{aligned} \tag{3-61}$$

The variable `niterCMP` is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. CFL_{loc} starts at 1.3 and increases by 30% each iteration until it reaches $1.3^9 \approx 10.6$. It remains there until iteration number 20 at which it starts to increase until it reaches approximately 106. A final increase after iteration number 40

then takes it to 1060. Equation 3-61 can, for some advanced flows, increase $\mathrm{CFL}_{\mathrm{loc}}$ too slowly or too quickly. $\mathrm{CFL}_{\mathrm{loc}}$ can then be tuned for the specific application.

For details about the CFL regulator, see Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*.

Nitsche Constraints

Some boundary conditions are implemented using Nitsche constraints. These boundary conditions include

- Wall — Slip, sliding walls, and moving walls (that is, walls with nonzero translational velocity).
- Periodic Flow Condition
- Flow Continuity

The formulation used in the Fluid Flow interfaces in single-phase flow interfaces corresponds to the Symmetric Interior Penalty Galerkin method (SIPG). The SIPG method can be regarded to satisfy the boundary conditions in an integral sense rather than pointwise. More information on SIPG can be found in Ref. 15.

In particular, the SIPG formulation includes a penalty parameter that must be large enough for the formulation to be coercive. The higher the value, the better the boundary condition is fulfilled, but a too high value results in an ill-conditioned equation system. The penalty parameter is implemented according to Ref. 16.

Particle Tracing in Fluid Flow

The Particle Tracing Module is available to assist with these types of modeling problems.

It is possible to model particle tracing with COMSOL Multiphysics provided that the impact of the particles on the flow field is negligible. First compute the flow field, and then, as an analysis step, calculate the motion of the particles. The motion of a particle is defined by Newton's second law

$$m\frac{d^2\mathbf{x}}{dt^2} = \mathbf{F}\left(t, \mathbf{x}, \frac{d\mathbf{x}}{dt}\right)$$

where $\mathbf{x}$ is the position of the particle, m the particle mass, and $\mathbf{F}$ is the sum of all forces acting on the particle. Examples of forces acting on a particle in a fluid are the drag force, the buoyancy force, and the gravity force. The drag force represents the force that a fluid exerts on a particle due to a difference in velocity between the fluid and the particle. It includes the viscous drag, the added mass, and the Basset history term. Several empirical expressions have been suggested for the drag force. One of those is the one proposed by Khan and Richardson (Ref. 13). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

$$\mathrm{Re}_p = \frac{|\mathbf{u} - \mathbf{u}_p| 2r\rho}{\mu}$$

where $\mathbf{u}$ is the velocity of the fluid, $\mathbf{u}_p$ the particle velocity, r the particle radius, ρ the fluid density, and μ the dynamic viscosity of the fluid. The empirical expression for the drag force according to Khan and Richardson is

$$\mathbf{F} = \pi r^2 \rho |\mathbf{u} - \mathbf{u}_p| (\mathbf{u} - \mathbf{u}_p)[1.84\mathrm{Re}_p^{-0.31} + 0.293\mathrm{Re}_p^{0.06}]^{3.45}$$

The model *Flow Past a Cylinder* (Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow**) demonstrates how to add and set up particle tracing in a plot group using the **Particle Tracing with Mass** node. It uses the predefined Khan–Richardson model for the drag force and neglects gravity and buoyancy forces.

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Theory for the Turbulent Flow Interfaces

The theory for the Single-Phase Flow, Turbulent Flow interfaces is described in this section:

- Turbulence Modeling
- The Algebraic yPlus Turbulence Model
- The L-VEL Turbulence Model
- The k-ε Turbulence Model
- The Realizable k-ε Turbulence Model
- The k-ω Turbulence Model
- The SST Turbulence Model
- The Low Reynolds Number k-ε Turbulence Model
- The Spalart–Allmaras Turbulence Model
- The v2-f Turbulence Model
- The Wilcox R-ω Turbulence Model
- The SSG-LRR Turbulence Model
- Theory for Turbulence in Porous Media
- Inlet Values for the Turbulence Length Scale and Turbulent Intensity
- Theory for Buoyancy-Induced Turbulence
- Theory for the Pressure, No Viscous Stress Boundary Condition
- Initial Values for Generate New Turbulence Model Interfaces
- Solvers for Turbulent Flow
- Pseudo Time Stepping for Turbulent Flow Models
- References for the Single-Phase Flow, Turbulent Flow Interfaces

Theory for the Single-Phase Flow Interfaces

Turbulence Modeling

Turbulence is a property of the flow field and it is characterized by a wide range of flow scales: the largest occurring scales, which depend on the geometry, the smallest, quickly fluctuating scales, and all the scales in between. The propensity for an isothermal flow to become turbulent is measured by the Reynolds number

$$\mathrm{Re} = \frac{\rho U L}{\mu} \tag{3-62}$$

where μ is the dynamic viscosity, ρ the density, and U and L are velocity and length scales of the flow, respectively. Flows with high Reynolds numbers tend to become turbulent. Most engineering applications belong to this category of flows.

The Navier–Stokes equations can be used for turbulent flow simulations, although this would require a large number of elements in order to capture the wide range of scales in the flow. An alternative approach is to divide the flow quantities into mean values and fluctuations. When solving for the mean-flow quantities, the effect of the fluctuations is modeled using a turbulence closure. The idea behind this approach is that solving the model for the turbulence closure is numerically less expensive than resolving all the turbulence scales. Different turbulence closures invoke different assumptions on the modeled fluctuations, resulting in various degrees of accuracy for different flow cases.

This module includes turbulence models based on the Reynolds-averaged Navier–Stokes (RANS) model, which is the model type most commonly used in industrial flow applications.

REYNOLDS-AVERAGED NAVIER–STOKES (RANS) EQUATIONS

The following assumes that the fluid is incompressible and Newtonian in which case the Navier–Stokes equations take the form:

$$\begin{gathered}\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F} \\ \rho\nabla\cdot\mathbf{u} = 0\end{gathered} \tag{3-63}$$

Once the flow has become turbulent, all quantities fluctuate in time and space. It is seldom worth the extreme computational cost to obtain detailed information about the fluctuations. An averaged representation often provides sufficient information about the flow.

The Reynolds-averaged representation of turbulent flows divides the flow quantities into an averaged value and a fluctuating part,

$$\phi = \bar{\phi} + \phi'$$

where ϕ can represent any scalar quantity of the flow. In general, the mean value can vary in space and time. This is exemplified in Figure 3-6, which shows time averaging of one component of the velocity vector for nonstationary turbulence. The unfiltered flow has a time scale Δt_1. After a time filter with width $\Delta t_2 >> \Delta t_1$ has been applied, there is a fluctuating part, u'_i, and an average part, U_i. Because the flow field also varies on a time scale longer than Δt_2, U_i is still time-dependent but is much smoother than the unfiltered velocity u_i.

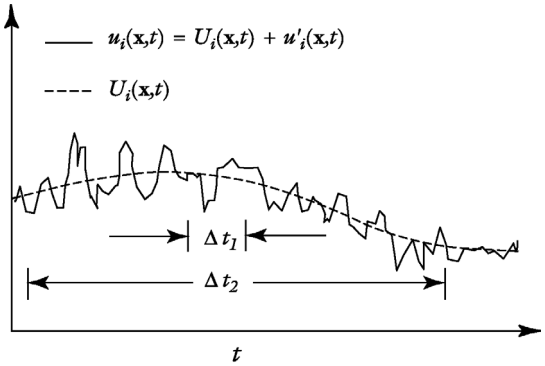

Figure 3-6: The unfiltered velocity component u_i, with a time scale Δt_1, and the averaged velocity component, U_i, with time scale Δt_2.

Decomposition of the flow field into an averaged part and a fluctuating part, followed by insertion into the Navier–Stokes equation, and averaging, gives the Reynolds-averaged Navier–Stokes (RANS) equations:

$$\rho\frac{\partial \mathbf{U}}{\partial t} + \rho\mathbf{U}\cdot\nabla\mathbf{U} + \nabla\cdot\overline{(\rho\mathbf{u}'\otimes\mathbf{u}')} = -\nabla P + \nabla\cdot\mu(\nabla\mathbf{U} + (\nabla\mathbf{U})^T) + \mathbf{F}$$
$$\rho\nabla\cdot\mathbf{U} = 0 \qquad (3\text{-}64)$$

where $\mathbf{U}$ is the averaged velocity field and $\otimes$ is the outer vector product. A comparison with Equation 3-63 indicates that the only difference is the appearance of the last term on the left-hand side of Equation 3-64. This term represents the interaction between the fluctuating parts of the velocity field and is called the Reynolds stress tensor. This means that to obtain the mean flow characteristics, information about the small-scale

structure of the flow is needed. In this case, that information is the correlation between fluctuations in all three directions.

EDDY VISCOSITY MODEL

The most common way to model turbulence is to assume that the turbulence is of a purely diffusive nature. The deviating part of the Reynolds stress is then expressed as

$$\rho(\overline{\mathbf{u}' \otimes \mathbf{u}'}) - \frac{\rho}{3}\text{trace}(\overline{\mathbf{u}' \otimes \mathbf{u}'})\mathbf{I} = -\mu_T(\nabla \mathbf{U} + (\nabla \mathbf{U})^T) \tag{3-65}$$

where μ_T is the *eddy viscosity*, also known as the turbulent viscosity. The spherical part can be rewritten as

$$\frac{\rho}{3}\text{trace}(\overline{\mathbf{u}' \otimes \mathbf{u}'})\mathbf{I} = \frac{2}{3}\rho k \tag{3-66}$$

where k is the turbulent kinetic energy. In simulations of incompressible flows, this term is included in the pressure, but when the absolute pressure level is of importance (in compressible flows, for example) this term must be explicitly included. A RANS model based on Equation 3-65 is referred to as Reynolds-averaged Navier–Stokes, eddy-viscosity model (RANS-EVM).

REYNOLDS STRESS MODEL

A more advanced approach is based on not assuming a particular form for the Reynolds stress tensor $\mathbf{R} = \overline{\mathbf{u}' \otimes \mathbf{u}'}$, but instead writing a transport equation for $\mathbf{R}$:

$$\rho\frac{\partial R_{ij}}{\partial t} + \rho U_k \frac{\partial R_{ij}}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\overline{\rho u'_i u'_j u'_k + p'(u'_i \delta_{jk} + u'_j \delta_{ik})} - \mu\frac{\partial R_{ij}}{\partial x_k}\right) = \tag{3-67}$$
$$-\rho\left(R_{ik}\frac{\partial U_j}{\partial x_k} + R_{jk}\frac{\partial U_i}{\partial x_k}\right) + \overline{p'\left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}\right)} - \overline{2\mu\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}}$$

This is a symmetric tensor equation that consists of six scalar equations. The production term has explicit form

$$P_{ij} = -\rho\left(R_{ik}\frac{\partial U_j}{\partial x_k} + R_{jk}\frac{\partial U_i}{\partial x_k}\right) \tag{3-68}$$

Half of its trace is the common production of turbulence kinetic energy $k = R_{kk}/2$

$$P = -\rho R_{ij}\frac{\partial U_i}{\partial x_j} \tag{3-69}$$

Of primary importance is the modeling of the pressure–strain correlation Π_{ij}:

$$\Pi_{ij} = p'\left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}\right) \tag{3-70}$$

which is responsible for the redistribution of the turbulence kinetic energy among the components of **R**. The turbulent diffusion **D** and turbulent dissipation ε_{ij} of **R** are usually modeled as

$$D_{ij} = \frac{\partial}{\partial x_k}\overline{(-\rho u'_i u'_j u'_k - p'(u'_i \delta_{jk} + u'_j \delta_{ik}))} = \frac{\partial}{\partial x_k}\left(\sigma^* \mu_T \frac{\partial R_{ij}}{\partial x_k}\right), \tag{3-71}$$

$$\rho\varepsilon_{ij} = \overline{2\mu \frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}} = \frac{2}{3}\rho\varepsilon\delta_{ij}$$

although more complicated approaches can be used. Here, σ^* is a modeling constant and ε is the scalar dissipation of turbulence kinetic energy. A RANS model based on Equation 3-67 is referred to as a Reynolds-averaged Navier–Stokes, Reynolds stress model (RANS-RSM).

TURBULENT COMPRESSIBLE FLOW

If the Reynolds average is applied to the compressible form of the Navier–Stokes equations, terms of the form

$$\overline{\rho' u'}$$

appear and need to be modeled. To avoid this, a density-based average, known as the Favre average, is introduced:

$$\tilde{u}_i = \frac{1}{\bar{\rho}} \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} \rho(\mathbf{x},\tau) u_i(\mathbf{x},\tau)\, d\tau \tag{3-72}$$

It follows from Equation 3-72 that

$$\bar{\rho}\tilde{u}_i = \overline{\rho u_i} \tag{3-73}$$

and a variable, u_i, is decomposed into a mass-averaged component, $\tilde{u}_i$, and a fluctuating component, u_i'', according to

$$u_i = \tilde{u}_i + u_i'' \tag{3-74}$$

Using Equation 3-73 and Equation 3-74 along with some modeling assumptions for compressible flows (Ref. 7), Equation 3-16 and Equation 3-17 can be written on the form

$$\begin{gathered}\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i)=0\\ \bar{\rho}\frac{\partial \tilde{u}_i}{\partial t}+\bar{\rho}\tilde{u}_j\frac{\partial \tilde{u}_i}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}\right)-\frac{2}{3}\mu\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}-\overline{\rho u_j'' u_i''}\right)+\bar{F}_i\end{gathered} \tag{3-75}$$

In RANS-EVM, the Favre-averaged Reynolds stress tensor is modeled using the same argument as for incompressible flows:

$$-\overline{\rho u_j'' u_i''}=\mu_T\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}\right)-\frac{2}{3}\left(\mu_T\frac{\partial \tilde{u}_k}{\partial x_k}+\bar{\rho}k\right)\delta_{ij}$$

where k is the turbulent kinetic energy. Comparing Equation 3-75 to its incompressible counterpart (Equation 3-64), it can be seen that except for the term

$$-(2/3)\bar{\rho}k\delta_{ij}$$

the compressible and incompressible formulations are exactly the same, except that the free variables are $\tilde{u}_i$ instead of

$$U_i=\bar{u}_i$$

In RANS-RSM, the Favre-averaged Reynolds stress tensor $\bar{\rho}\mathbf{R}=\overline{\rho\mathbf{u}''\otimes\mathbf{u}''}$ is determined using Equation 3-67, Equation 3-70 and Equation 3-71, where

$$\rho\rightarrow\bar{\rho},\ U_i\rightarrow\tilde{u}_i,\ u'_i\rightarrow u''_i$$

More information about modeling turbulent compressible flows can be found in Ref. 1 and Ref. 7.

The turbulent transport equations are used in their fully compressible formulations (Ref. 8).

The Algebraic yPlus Turbulence Model

The algebraic yPlus turbulence model is an algebraic turbulence model based on the distance to the nearest wall. The model is based on Prandtl's mixing-length theory and is suitable for internal flows. It is less mesh sensitive than transport-equation models

like Spalart–Allmaras or the k-ε model. In what follows, let y be the coordinate normal to the wall, and U the velocity parallel to the wall. Using a mixing length formulation, the balance for the shear stress in the wall layer may be approximated as

$$\left(\mu + \rho l_{\text{mix}}^2 \left|\frac{\partial U}{\partial y}\right|\right)\frac{\partial U}{\partial y} = \rho u_\tau^2$$

which, expressed on dimensionless form, reduces to

$$\left(1 + l_{\text{mix}}^{+2}\left|\frac{\partial u^+}{\partial y^+}\right|\right)\frac{\partial u^+}{\partial y^+} = 1 \tag{3-76}$$

where $y^+ = y u_\tau/\nu$, $u^+ = U/u_\tau$ and $u_\tau = \sqrt{\tau_w/\rho}$ is the friction velocity. Close to the wall, the mixing length must be zero such that $u^+ = y^+$, and far away from the wall, $l_{\text{mix}}^+ \approx \kappa y^+$ such that $u^+ = (1/\kappa)\log(y^+) + B$. To obtain the correct behavior, the mixing length is chosen to be

$$l_{\text{mix}}^+ = \begin{cases} 0 & y^+ \le y^* \\ \kappa(y^+ - y^*) & y^+ > y^* \end{cases} \tag{3-77}$$

where y^* is to be determined. Inserting Equation 3-77 into Equation 3-76

$$\frac{\partial u^+}{\partial y^+} = \begin{cases} 1 & y^+ \le y^* \\ \dfrac{\sqrt{1 + 4\kappa^2(y^+ - y^*)^2} - 1}{2\kappa^2(y^+ - y^*)^2} & y^+ > y^* \end{cases} \tag{3-78}$$

Integrating Equation 3-78

$$u^+ = \begin{cases} y^+ & y^+ \le y^* \\ y^* + \dfrac{1 - \sqrt{1 + 4\kappa^2(y^+ - y^*)^2}}{2\kappa^2(y^+ - y^*)} & \\ \quad + \dfrac{1}{\kappa}\log\left(\sqrt{1 + 4\kappa^2(y^+ - y^*)^2} + 2\kappa(y^+ - y^*)\right) & y^+ > y^* \end{cases} \tag{3-79}$$

For large values of y^+, Equation 3-79 reduces to

$$u^+ = \frac{1}{\kappa}\log(y^+) + \frac{1}{\kappa}(\log(4e\kappa) - 1) + y^*$$

Comparing the above expression with the logarithmic law of the wall

$$u^+ = \frac{1}{\kappa}\log(y^+) + B$$

the value of the constant y^* is obtained as

$$y^* = B - \frac{1}{\kappa}(\log(4\kappa) - 1)$$

The dimensionless effective viscosity can be evaluated from

$$\nu^+ = \begin{cases} 1 & y^+ \le y^* \\ 1 + \kappa^2(y^+ - y^*)^2\left|\frac{\partial u^+}{\partial y^+}\right| = \frac{1 + \sqrt{1 + 4\kappa^2(y^+ - y^*)^2}}{2} & y^+ > y^* \end{cases} \quad (3\text{-}80)$$

This requires the local value of y^+, which is obtained from the Reynolds number

$$\mathrm{Re} = \frac{Uy}{\nu} = \frac{U}{u_\tau}\frac{yu_\tau}{\nu} = u^+y^+ =$$

$$\begin{cases} y^{+2} & y^+ \le y^* \\ y^+\left(y^* + \frac{1 - \sqrt{1 + 4\kappa^2(y^+ - y^*)^2}}{2\kappa^2(y^+ - y^*)} + \frac{1}{\kappa}\log\left(\sqrt{1 + 4\kappa^2(y^+ - y^*)^2} + 2\kappa(y^+ - y^*)\right)\right) & y^+ > y^* \end{cases} \quad (3\text{-}81)$$

The nonlinear algebraic Equation 3-81 has to be solved at each node point to evaluate the effective viscosity from Equation 3-80. The local Reynolds number $\mathrm{Re} = Uy/\nu$ is formed with the local absolute value of the velocity and the distance to the nearest wall. This implicitly assumes that the main flow direction is parallel to the wall.

WALL DISTANCE

The wall distance, y is provided by a mathematical Wall Distance interface that is included when using the Algebraic yPlus model. The solution to the wall distance

equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITION

Low Reynolds Number Wall Treatment

The Algebraic yPlus turbulence model is consistent with a no slip boundary condition, that is $\mathbf{u} = \mathbf{0}$. Since the turbulence model is algebraic, no additional boundary condition is needed. This boundary conditions is applied for **Wall Treatment** equal to **Low Re**.

The low-Reynolds-number formulation of the Algebraic yPlus model can be considered to be well resolved at a wall when the wall resolution in viscous units

$$\Delta_w^+ = \rho u_\tau h_w / \mu \sim 1 \tag{3-82}$$

where the resolution height is based on the distance between the first computational node inside the domain and the wall. u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \tag{3-83}$$

and is available as the postprocessing variable $u_{\tau w}$ (`u_tauWall`). Also, the boundary variable **Distance to cell center in viscous units**, l_c^+ (`lplus_cc`), is available to ensure that the mesh is fine enough. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell, thus $l_c^+ = 0.5\,\Delta_w^+$ and according to Equation 3-82 l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

The postprocessing variable **Wall resolution in viscous units**, Δ_w^+ (`Delta_wPlus`), is available.

Automatic Wall Treatment

The default boundary treatment for Algebraic yPlus is the **Automatic** wall treatment. The automatic wall treatment assumes that there is a small gap, $\delta_w = h_w/2$, between the computational domain and the physical wall. Here, h_w is the height of the mesh cell adjacent to the wall (see Figure 3-7).

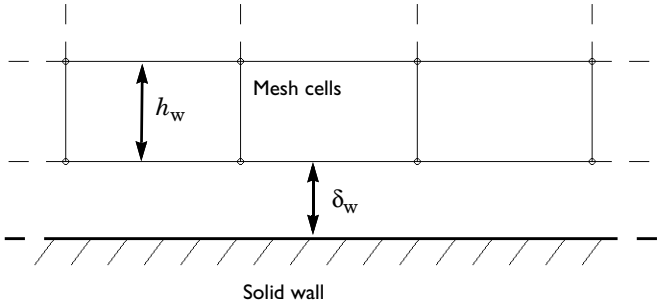

Figure 3-7: The computational domain is located a distance δ_w from the wall.

The boundary conditions for the velocity is a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \mathbf{K} - (\mathbf{n} \cdot \mathbf{K} \cdot \mathbf{n})\mathbf{n} = -\rho u_\tau^2 \frac{\mathbf{u}}{|\mathbf{u}|}$$

where

$$\mathbf{K} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

and

$$u_\tau = \frac{\mathbf{u}}{u^+}$$

The postprocessing variable for friction velocity u_τ is based on the effective traction at the wall and is available as $u_{\tau w}$ (`u_tauWall`). The wall traction using $u_{\tau w}$ is available as postprocessing variable `T_trac`. The automatic wall treatment tends to the low-Reynolds-number formulation when h_w tends to zero, and it becomes a wall function formulation when the resolution in viscous units

$$\Delta_w^+ = \frac{u_{\tau w}\delta_w}{\nu}$$

increases. The resolution in viscous units $\Delta_w{}^+$ is available as a postprocessing variable, `Delta_wPlus`. The resolution height is based on the distance of the first computational node (which is on the wall) from the imaginary lift-off wall.

See also Wall for boundary condition details.

In the *COMSOL Multiphysics Reference Manual:*

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The L-VEL Turbulence Model

The *L-VEL (Length-VELocity) turbulence model* is an algebraic turbulence model often used in electronic cooling applications. It is less mesh sensitive than transport-equation models like Spalart–Allmaras or the k-ε model. It was developed by Agonafer and others (Ref. 24) for internal flows and uses an extension of the logarithmic law of the wall which applies all the way down to the wall

$$y^+ = u^+ + \frac{1}{E}\left(e^{\kappa u^+} - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6} - \frac{(\kappa u^+)^4}{24}\right) \tag{3-84}$$

where $y^+ = yu_\tau/\nu$, $u^+ = U/u_\tau$, U is the local flow speed, y is the distance to the nearest wall, ν is the kinematic viscosity, u_τ is the friction velocity, κ is the von Kármán constant, and $E = 8.6$ is another constant needed to fit the logarithmic law of the wall. The shear stress in the wall layer is given by

$$\rho(\nu + \nu_T)\frac{\partial U}{\partial y} = \rho u_\tau^2 \Rightarrow 1 + \frac{\nu_T}{\nu} = \frac{u_\tau^2}{\nu}\frac{1}{\partial U/\partial y} = \frac{1}{\partial(U/u_\tau)/\partial(yu_\tau/\nu)} \Rightarrow$$

$$\nu^+ = \frac{1}{\partial u^+/\partial y^+}$$

Differentiating Equation 3-84 with respect to y^+, the dimensionless effective viscosity is obtained as

$$\nu^+ = 1 + \frac{\kappa}{E}\left(e^{\kappa u^+} - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6}\right) \tag{3-85}$$

If the local value of u^+ is known, the effective viscosity can be evaluated from Equation 3-85. The value of u^+ is obtained by forming a local Reynolds number

$$\begin{aligned}\mathrm{Re} &= \frac{Uy}{\nu} = \frac{U}{u_\tau}\frac{yu_\tau}{\nu} = u^+y^+ = \\ &= u^+\left(u^+ + \frac{1}{E}\left(e^{\kappa u^+} - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6} - \frac{(\kappa u^+)^4}{24}\right)\right)\end{aligned} \tag{3-86}$$

where the last expression follows from Equation 3-84. Hence, the nonlinear algebraic Equation 3-86 has to be solved at each node point to evaluate the effective viscosity. The local Reynolds number $\mathrm{Re} = Uy/\nu$ is formed with the local absolute value of the velocity and the distance to the nearest wall. This implicitly assumes that the main flow direction is parallel to the wall.

WALL DISTANCE

The wall distance, y is provided by a mathematical Wall Distance interface that is included when using the L-VEL model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITION

Low Reynolds Number Wall Treatment

The L-VEL turbulence model is consistent with a no slip boundary condition, that is $\mathbf{u} = \mathbf{0}$. Since the turbulence model is algebraic, no additional boundary condition is needed. This boundary conditions is applied for **Wall Treatment** equal to **Low Re**.

The low-Reynolds-number formulation of The L-VEL model can be considered to be well resolved at a wall when the wall resolution in viscous units

$$\Delta_w^+ = \rho u_\tau h_w/\mu \sim 1 \tag{3-87}$$

where the resolution height is based on the distance between the first computational node inside the domain and the wall. u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \tag{3-88}$$

and is available as the postprocessing variable $u_{\tau w}$ (`u_tauWall`). Also, the boundary variable **Distance to cell center in viscous units**, l_c^+ (`lplus_cc`), is available to ensure that the mesh is fine enough. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell, thus $l_c^+ = 0.5\Delta_w^+$ and according to Equation 3-87 l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

The postprocessing variable **Wall resolution in viscous units**, Δ_w^+ (`Delta_wPlus`), is available.

Automatic Wall Treatment

The default boundary treatment for Algebraic yPlus is the **Automatic** wall treatment. The details are described in Wall Boundary Condition for The Algebraic yPlus Turbulence Model.

See also Wall for boundary condition details.

In the *COMSOL Multiphysics Reference Manual:*

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The k-ε Turbulence Model

The k-ε model is one of the most used turbulence models for industrial applications. This module includes the standard k-ε model (Ref. 1). The model introduces two additional transport equations and two dependent variables: the turbulent kinetic energy, k, and the turbulent dissipation rate, ε. The turbulent viscosity is modeled as

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon} \tag{3-89}$$

where C_μ is a model constant.

The transport equation for k reads:

$$\rho\frac{\partial k}{\partial t} + \rho\mathbf{u}\cdot\nabla k = \nabla\cdot\left(\left(\mu + \frac{\mu_T}{\sigma_k}\right)\nabla k\right) + P_k - \rho\varepsilon \tag{3-90}$$

where the production term is

$$P_k = \mu_T\left(\nabla\mathbf{u}:(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}(\nabla\cdot\mathbf{u})^2\right) - \frac{2}{3}\rho k\nabla\cdot\mathbf{u} \tag{3-91}$$

The transport equation for ε reads

$$\rho\frac{\partial \varepsilon}{\partial t} + \rho\mathbf{u}\cdot\nabla\varepsilon = \nabla\cdot\left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\nabla\varepsilon\right) + C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} \tag{3-92}$$

The model constants in Equation 3-89, Equation 3-90, and Equation 3-92 are determined from experimental data (Ref. 1) and the values are listed in Table 3-4.

TABLE 3-4: MODEL CONSTANTS.

CONSTANT	VALUE
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3

MIXING LENGTH LIMIT

Equation 3-90 and Equation 3-92 cannot be implemented directly as written. There is, for example, nothing that prevents division by zero. The equations are instead implemented as suggested in Ref. 10. The implementation includes an upper limit on the mixing length, $l_{\text{mix}}^{\text{lim}}$:

$$l_{\text{mix}} = \max\left(C_\mu\frac{k^{3/2}}{\varepsilon}, l_{\text{mix}}^{\text{lim}}\right) \tag{3-93}$$

The mixing length is used to calculated the turbulent viscosity. $l_{\text{mix}}^{\text{lim}}$ should not be active in a converged solution but is merely a tool to obtain convergence.

REALIZABILITY CONSTRAINTS

The eddy-viscosity model of the Reynolds stress tensor can be written

$$\rho\overline{u_i u_j} = -2\mu_T S_{ij} + \frac{2}{3}\rho k\delta_{ij}$$

where δ_{ij} is the Kronecker delta and S_{ij} is the strain-rate tensor. The diagonal elements of the Reynolds stress tensor must be nonnegative, but calculating μ_T from Equation 3-89 does not guarantee this. To assert that

$$\rho\overline{u_i u_i} \geq 0 \quad \forall i$$

the turbulent viscosity is subjected to a realizability constraint. The constraint for 2D and 2D axisymmetry without swirl is:

$$\mu_T \leq \frac{\rho k\sqrt{2}}{3\sqrt{S_{ij}S_{ij}}} \tag{3-94}$$

and for 3D and 2D axisymmetry with swirl flow it reads:

$$\mu_T \leq \frac{\rho k}{\sqrt{6}\sqrt{S_{ij}S_{ij}}} \tag{3-95}$$

Combining equation Equation 3-94 with Equation 3-89 and the definition of the mixing length gives a limit on the mixing length scale:

$$l_{\text{mix}} \leq \frac{\sqrt{2}}{3}\frac{\sqrt{k}}{\sqrt{S_{ij}S_{ij}}} \tag{3-96}$$

Equivalently, combining Equation 3-95 with Equation 3-89 and Equation 3-93 gives:

$$l_{\text{mix}} \leq \frac{1}{\sqrt{6}}\frac{\sqrt{k}}{\sqrt{S_{ij}S_{ij}}} \tag{3-97}$$

This means there are two limitations on l_{mix}: the realizability constraint and the imposed limit via Equation 3-93.

The effect of not applying a realizability constraint is typically excessive turbulence production. The effect is most clearly visible at stagnation points. To avoid such artifacts, the realizability constraint is always applied for the RANS models. More details can be found in Ref. 4, Ref. 5, and Ref. 6.

MODEL LIMITATIONS

The k-ε turbulence model relies on several assumptions, the most important of which is that the Reynolds number is high enough. It is also important that the turbulence is in equilibrium in boundary layers, which means that production equals dissipation. These assumptions limit the accuracy of the model because they are not always true. It

does not, for example, respond correctly to flows with adverse pressure gradients and can result in under-prediction of the spatial extent of recirculation zones (Ref. 1). Furthermore, in simulations of rotating flows, the model often shows poor agreement with experimental data (Ref. 2). In most cases, the limited accuracy is a fair tradeoff for the amount of computational resources saved compared to using more complicated turbulence models.

WALL FUNCTIONS

The flow close to a solid wall is for a turbulent flow very different from the free stream. This means that the assumptions used to derive the k-ε model are not valid close to walls. While it is possible to modify the k-ε model so that it describes the flow in wall regions (see The Low Reynolds Number k-$\mathcal{E}$ Turbulence Model), this is not always desirable because of the very high resolution requirements that follow. Instead, analytical expressions are used to describe the flow near the walls. These expressions are known as wall functions.

When using wall functions in COMSOL Multiphysics, a theoretical lift-off from the physical wall is assumed as shown in Figure 3-7. Expressed in viscous units, the wall lift-off is defined as

$$\delta_w^+ = \max\left(\frac{h_w}{2}\frac{\rho C_\mu^{1/4}\sqrt{k}}{\mu}, 11.06\right)$$

The first argument is derived from the law of the wall. The second argument is the distance from the wall, in viscous units, where the logarithmic layer meets the viscous sublayer (or rather would meet it if there were no buffer layer in between). This lower limit ensures that the wall functions remain nonsingular for all Reynolds numbers.

The wall lift-off, δ_w, is defined as

$$\delta_w = \frac{\delta_w^+ \mu}{\rho u_\tau}$$

where the friction velocity, u_τ, is defined by

$$u_\tau = \max\left(C_\mu^{1/4}\sqrt{k}, \frac{\|\mathbf{u}\|}{u^+}\right)$$

$$u^+ = \frac{1}{\kappa_v}\log(\delta_w^+) + B$$

where in turn, κ_v, is the von Kármán constant (default value 0.41) and B is a constant that by default is set to 5.2. The two arguments for u_τ are under some additional assumptions theoretically identical in the logarithmic layer (Ref. 1), but deviate in stagnation points and when the local Reynolds number becomes low. The definition of δ_w is such that it becomes $h_w/2$ (or somewhat smaller if $\|\mathbf{u}\| > C_\mu^{1/4}\sqrt{k}\,u^+$) when $\delta_w^+ > 11.06$, but it can become many times larger when the lower limit for δ_w^+, 11.06, takes effect.

The boundary conditions for the velocity is a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \mathbf{K} - (\mathbf{n} \cdot \mathbf{K} \cdot \mathbf{n})\mathbf{n} = -\rho u_\tau \frac{\mathbf{u}}{u^+}$$

where

$$\mathbf{K} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

is the viscous stress tensor.

The turbulent kinetic energy is subject to a homogeneous Neumann condition $\mathbf{n} \cdot \nabla k = 0$ and the boundary condition for ε reads:

$$\varepsilon = \frac{C_\mu^{3/4} k^{3/2}}{\kappa_v \delta_w}$$

See Ref. 10 and Ref. 11 for further details.

The postprocessing variable for the friction velocity $u_{\tau w}$ (`u_tauWall`) is based on the effective traction at the wall and is defined as

$$u_{\tau w} = \sqrt{u_\tau \frac{|\mathbf{u}|}{u^+}}$$

while the postprocessing variable for the wall resolution Δ_w^+ (`Delta_wPlus`) is based on $u_{\tau w}$ and is defined as

$$\Delta_w^+ = \max\left(\frac{\rho}{\mu}\frac{h_w}{2}u_{\tau w}, 11.06\right)$$

The resolution height is based on the distance of the first computational node (which is on the wall) from the imaginary lift-off wall. The wall traction using $u_{\tau w}$ is available as postprocessing variable `T_trac`.

Wall functions give reasonable predictions as long as Δ_w^+ is lower than some upper limit that depends on the turbulent Reynolds number (Ref. 29). The upper limit is hardly ever lower than 50, and in many practical applications as high as a few hundred. Highest accuracy is obtained if Δ_w^+ is also everywhere larger than 25, which approximately corresponds to the beginning of the logarithmic layer. It can also be worthwhile to check that δ_w is small compared to the dimensions of the geometry, especially if $\Delta_w^+ = 11.06$ for a significant fraction of the wall area.

WALL FUNCTIONS FOR ROUGH WALLS

The physics interfaces Wall and Interior Wall have an option to apply wall roughness by modifying the wall functions. Cebeci (Ref. 22) suggested a model which adjusts the friction velocity for surface roughness,

$$u_\tau = \frac{|\mathbf{u}|}{\frac{1}{\kappa_v}\ln\delta_w^+ + B - \Delta B} \tag{3-98}$$

where

$$\Delta B = \begin{cases} 0 & k_s^+ \le 2.25 \\ \frac{1}{\kappa_v}\ln\left[\frac{k_s^+ - 2.25}{87.75} + C_s k_s^+\right]\sin[0.4258(\ln k_s^+ - 0.811)] & 2.25 \le k_s^+ \le 90 \\ \frac{1}{\kappa_v}\ln(1 + C_s k_s^+) & k_s^+ \ge 90 \end{cases}$$

k_s^+ is the roughness height in viscous units,

$$k_s^+ = \frac{\rho C_\mu^{1/4}\sqrt{k}}{\mu} k_s$$

The roughness height, k_s, is the peak-to-peak value of the surface variations and the wall is relocated to their mean level.

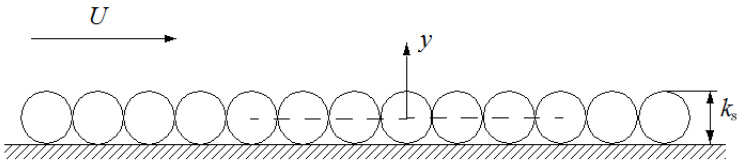

Figure 3-8: Definitions of the roughness height and the modified wall location.

Hence, when Equation 3-98 is used the lift-off is modified according to,

$$\delta_w^+ = \max\{11.06,\ k_s^+/2,\ h^+/2\}$$

where h^+ is the height of the boundary mesh cell in viscous units. C_s is a parameter that depends on the shape and distribution of the roughness elements. When the turbulence parameters κ_v and B have the values 0.41 and 5.2, respectively, and $C_s = 0.26$, k_s corresponds to the *equivalent sand roughness height*, k_{seq}, as introduced by Nikuradse (Ref. 23). A few characteristic values of the equivalent sand roughness height are given in Table 3-5 below,

TABLE 3-5: EQUIVALENT SAND ROUGHNESS HEIGHTS k_{seq}.

SURFACE TYPE	EQUIVALENT SAND ROUGHNESS HEIGHT
Steel, new	50 µm
Galvanized steel	0.13 mm
Riveted steel	0.9-9 mm
Cast iron, new	0.25 mm
Galvanized iron	0.15-0.30 mm
Cast iron, rusted	1.0-1.5 mm
Bituminized steel or iron, new	30-50 µm
Glass	0.3 µm
Drawn tubing	1.5 µm
Wood, new	0.5 mm
Concrete, new	0.3-3 mm

Use other values of the roughness parameter C_s and roughness height k_s to specify generic surface roughnesses.

INITIAL VALUES

The default initial values for a stationary simulation are (Ref. 10),

$$\mathbf{u} = 0$$
$$p = 0$$
$$k = \left(\frac{10 \cdot \mu}{\rho(0.1 \cdot l_{mix}^{lim})}\right)^2$$
$$\varepsilon = \frac{C_\mu k_{init}^{3/2}}{0.1 \cdot l_{mix}^{lim}}$$

where $l_{\text{mix}}^{\text{lim}}$ is the mixing length limit. For time-dependent simulations, the initial value for k is instead

$$k = \left(\frac{\mu}{\rho(0.1 \cdot l_{\text{mix}}^{\text{lim}})}\right)^2$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The k-ε equations are derived under the assumption that the flow has a high enough Reynolds number. If this assumption is not fulfilled, both k and ε have very small magnitudes and behave chaotically in the manner that the relative values of k and ε can change by large amounts due to small changes in the flow field.

A time-dependent simulation of a turbulent flow can include a period when the flow is not fully turbulent. A typical example is the startup phase when for example an inlet velocity or a pressure difference is gradually increased. To sort out numerical fluctuations in k and ε during such periods, the default time-dependent solver for the k-ε model employs unscaled absolute tolerances for k and ε. The tolerances are set to

$$\begin{aligned} k_{\text{scale}} &= (0.1 U_{\text{scale}})^2 \\ \varepsilon_{\text{scale}} &= 0.09 k_{\text{sclae}}^{3/2} / (L_{\text{fact}} \cdot l_{\text{bb, min}}) \end{aligned} \tag{3-99}$$

where U_{scale} and L_{fact} are input parameters available in the Advanced Settings section of the physics interface node. Their default values are 1 m/s and 0.035 respectively. $l_{\text{bb,min}}$ is the shortest side of the geometry bounding box. Equation 3-99 is closely related to the expressions for k and ε on inlet boundaries (see Equation 3-255).

The practical implication of Equation 3-99 is that variations in k and ε smaller than k_{scale} and $\varepsilon_{\text{scale}}$, respectively, are regarded as numerical noise.

The Realizable k-ε Turbulence Model

The Realizable k-ε turbulence model (Ref. 14) is an extension to the standard k-ε model with built-in realizability conditions,

$$\begin{aligned} \overline{u_i^2} &\geq 0 \\ \frac{\overline{u_i u_j}^2}{\overline{u_i^2}\,\overline{u_j^2}} &\leq 1 \end{aligned} \tag{3-100}$$

The transport equation for the turbulent kinetic energy is the same as for the standard k-ε model, Equation 3-90, while Equation 3-101 is solved for the turbulent dissipation rate,

$$\rho\frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\nabla \varepsilon\right) + C_1 \rho S \varepsilon - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}} \tag{3-101}$$

where,

$$C_1 = \max\left\{0.43, \frac{\eta}{5+\eta}\right\}, \quad \eta = \frac{Sk}{\varepsilon}, \quad S = \sqrt{2S_{ij}S_{ij}}, \quad S_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \tag{3-102}$$

The turbulent viscosity is given by Equation 3-89, but C_μ is not constant for the realizable k-ε model,

$$C_\mu = \frac{1}{A_0 + A_s U^{(*)}\frac{k}{\varepsilon}} \tag{3-103}$$

with,

$$A_s = \sqrt{6}\cos\left(\frac{1}{3}\operatorname{acos}(\sqrt{6}W)\right), \quad W = \frac{2\sqrt{2}S_{ij}S_{jk}S_{ki}}{S^3} \tag{3-104}$$

and,

$$U^{(*)} = \sqrt{S_{ij}S_{ij} + \Omega_{ij}\Omega_{ij}}, \quad \Omega_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial \bar{u}_j}{\partial x_i}\right) \tag{3-105}$$

S_{ij} and Ω_{ij} are the mean strain- and rotation-rate tensors respectively. The default constants for the Realizable k-ε model are,

$$C_{\varepsilon 2} = 1.9 \quad A_0 = 4 \quad \sigma_k = 1 \quad \sigma_\varepsilon = 1.2 \tag{3-106}$$

MODEL PROPERTIES

Compared to the standard k-ε model, the realizable k-ε model yields better predictions for certain flows. One example is the round jet, for which the standard k-ε model overestimates the spreading rate. In general, since the realizability conditions in Equation 3-100 are approached asymptotically, the turbulence characteristics are more

consistent than for the standard k-ε model. The realizable k-ε model uses wall functions and has the same default initial conditions and scalings as the standard k-ε model (see Wall Functions, Initial Values and Scaling for Time-Dependent Simulations).

The k-ω Turbulence Model

The k-ω model solves for the turbulent kinetic energy, k, and for the dissipation per unit turbulent kinetic energy, ω. ω is also commonly know as the specific dissipation rate. The CFD Module has the Wilcox revised k-ω model (Ref. 1)

$$\begin{aligned}\rho\frac{\partial k}{\partial t}+\rho\mathbf{u}\cdot\nabla k &= P_k-\rho\beta^* k\omega+\nabla\cdot((\mu+\sigma^*\mu_T)\nabla k)\\ \rho\frac{\partial \omega}{\partial t}+\rho\mathbf{u}\cdot\nabla\omega &= \alpha\frac{\omega}{k}P_k-\rho\beta\omega^2+\nabla\cdot((\mu+\sigma\mu_T)\nabla\omega)\end{aligned} \tag{3-107}$$

where

$$\mu_T = \rho\frac{k}{\omega} \tag{3-108}$$

$$\alpha=\frac{13}{25}\quad \beta=\beta_0 f_\beta\quad \beta^*=\beta_0^* f_{\beta\cdot}\quad \sigma=\frac{1}{2}\quad \sigma^*=\frac{1}{2}$$

$$\beta_0=\frac{9}{125}\quad f_\beta=\frac{1+70\chi_\omega}{1+80\chi_\omega}\quad \chi_\omega=\left|\frac{\Omega_{ij}\Omega_{jk}S_{ki}}{(\beta_0^*\omega)^3}\right|$$

$$\beta_0^*=\frac{9}{100}\quad f_{\beta\cdot}=\begin{cases}1 & \chi_k\le 0\\ \dfrac{1+680\chi_k^2}{1+400\chi_k^2} & \chi_k>0\end{cases}\quad \chi_k=\frac{1}{\omega^3}(\nabla k\cdot\nabla\omega) \tag{3-109}$$

where in turn Ω_{ij} is the mean rotation-rate tensor

$$\Omega_{ij}=\frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j}-\frac{\partial \overline{u}_j}{\partial x_i}\right)$$

and S_{ij} is the mean strain-rate tensor

$$S_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)$$

P_k is given by Equation 3-91. The following auxiliary relations for the dissipation, ε, and the turbulent mixing length, l_*, are also used:

$$\varepsilon = \beta^* \omega k \quad l_{mix} = \frac{\sqrt{k}}{\omega} \tag{3-110}$$

MIXING LENGTH LIMIT AND REALIZABILITY CONSTRAINTS

The implementation of the k-ω model relies on the same concepts as the k-ε model (Ref. 10). This means that the following approximations have been used:

$$\frac{\omega}{k} \approx \frac{\rho}{\max(\mu_T, eps)}$$

$$\frac{1}{\omega} = \frac{\sqrt{k}}{\omega\sqrt{k}} = \frac{l_{mix}}{\sqrt{k}} = l_{mix}\left(\frac{\rho l_{mix}}{\mu_T}\right) \approx \frac{l_{mix}^2 \rho}{\max(\mu_T, eps)}$$

$$l_{mix} = \min\left(\frac{\sqrt{k}}{\omega}, l_{mix}^{lim}, l_r\right)$$

where l_r is the limit given by the realizability constraints (Equation 3-96 and Equation 3-97).

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. For the specific dissipation, these solutions read

$$\omega_{visc} = \frac{6\nu}{\beta_0 \delta_w^2} \quad \omega_{log} = \frac{u_\tau}{\sqrt{\beta_0^*}\kappa_v \delta_w} \tag{3-111}$$

The corresponding expressions for the velocity is

$$u_\tau^{\text{visc}} = \sqrt{\frac{\nu U_\parallel}{\delta_w}} \quad u_\tau^{\log} = \frac{U_\parallel}{\frac{1}{\kappa_v}\log(\delta_w^+) + B} \tag{3-112}$$

where δ_w is the distance to the nearest wall, κ_v, is the von Kármán constant (default value 0.41), $U_\parallel$ is the velocity parallel to the wall, and B is a constant that by default is set to 5.2. Menter and others (Ref. 9) suggested the following smooth blending expressions for ω and u_τ:

$$\omega = \sqrt{\omega_{\text{visc}}^2 + \omega_{\log}^2} \tag{3-113}$$

and

$$u_\tau = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u_\tau^{\log})^4} \tag{3-114}$$

These expressions can be combined with the lift-off concept shown in Figure 3-7 which gives $\delta_w = h_w/2$. The wall condition for ω is given by Equation 3-113 and the conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \mathbf{K} - (\mathbf{n} \cdot \mathbf{K} \cdot \mathbf{n})\mathbf{n} = -\rho u_\tau \frac{\mathbf{u}}{u^+} \tag{3-115}$$

The k-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all $\delta_w{}^+$.

The system given by Equation 3-98 through Equation 3-115 are, however, nonlinear in u_τ and not very stable. To circumvent this, a variable $u^{*,\log}$ is introduced (see Ref. 10 and Ref. 11) such that

$$u^{*,\log} = \sqrt[4]{\beta_0^*}\sqrt{k} \tag{3-116}$$

This is then used in an alternative expression for the friction velocity:

$$u^* = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u^{*,\log})^4} \tag{3-117}$$

Equation 3-117 is in turn is used to calculate an alternative dimensionless wall distance

$$\delta_w^* = \frac{u^* \delta_w}{\nu} \tag{3-118}$$

Equation 3-117 is used instead of u_τ in the expression for ω_{log} and Equation 3-118 is used instead of δ_w^+ in the expression for u_τ^{log}. The traction condition in Equation 3-115 is replaced by

$$\mathbf{n} \cdot \mathbf{K} - (\mathbf{n} \cdot \mathbf{K} \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^+} \tag{3-119}$$

Observe that the variable $u^+ = |\mathbf{u}|/u_\tau$ is based on u_τ from Equation 3-114.

The postprocessing variable for friction velocity $u_{\tau w}$ (`u_tauWall`) is based on the effective traction at the wall and is defined as

$$u_{\tau w} = \sqrt{u_\tau u^*}$$

while the postprocessing variable for the resulting wall resolution Δ_w^+ (`Delta_wPlus`) is based on $u_{\tau w}$ and is defined as

$$\Delta_w^+ = \frac{u_{\tau w}\delta_w}{\nu}$$

The resolution height is based on the distance of the first computational node (which is on the wall) from the imaginary lift-off wall.

Wall Functions

When **Wall Treatment** is set to Wall functions, wall boundaries are treated with the same type of boundary conditions as for the k-ε model (see Wall Functions) with C_μ replaced by β_0^* and the boundary condition for ω given by

$$\omega_w = \frac{\rho k}{\kappa \delta_w^+ \mu} \tag{3-120}$$

Low Reynolds Number

The k-ω turbulence model can be integrated all the way down to the wall and is consistent with the no-slip condition $\mathbf{u} = 0$. Since all velocities must disappear on the wall, so must k. Hence, $k = 0$ on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_w \to 0} \omega = \frac{6\mu}{\rho \beta_0 l_w^2} \tag{3-121}$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-121 (using the variable ω_w, which

only exists in those cells). Accurate solutions in the near-wall region require that the wall resolution in viscous units

$$\Delta_w^+ = \rho u_\tau h_w / \mu \sim 1 \tag{3-122}$$

where the resolution height is based on the distance between the first computational node inside the domain and the wall. u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \tag{3-123}$$

and is available as the postprocessing variable $u_{\tau w}$ (`u_tauWall`). Also, the boundary variable **Distance to cell center in viscous units**, l_c^+ (`lplus_cc`), is available to ensure that the mesh is fine enough. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell, thus $l_c^+ = 0.5\Delta_w^+$ and according to Equation 3-122 l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

Since the ω_w requires the wall distance, a wall distance equation must be solved prior to solving a k-ω model with low-Reynolds-number wall treatment.

The postprocessing variable **Wall resolution in viscous units**, Δ_w^+ (`Delta_wPlus`), is available.

INITIAL VALUES

The default initial values are the same as for the k-ε model (see Initial Values) but with the initial value of ω given by

$$\omega_{init} = \frac{\sqrt{k_{init}}}{0.1 \cdot l_{mix}^{lim}}$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The k-ω model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations) except that the scale for ω is given by

$$\omega_{scale} = \frac{\sqrt{k_{scale}}}{L_{fact} \cdot l_{bb,\,min}}$$

MODEL PROPERTIES

The k-ω model can in many cases give results that are superior to those obtained with the k-ε model (Ref. 1). It behaves, for example, much better for flat plate flows with adverse or favorable pressure gradients. However, there are two main drawbacks. The first is that the k-ω model can display a relatively strong sensitivity to free stream inlet values of ω. The other is that the k-ω model is numerically less robust than the k-ε model.

The SST Turbulence Model

To combine the superior behavior of the k-ω model in the near-wall region with the robustness of the k-ε model, Menter (Ref. 18) introduced the SST (Shear Stress Transport) model which interpolates between the two. The version of the SST model in the CFD Module includes a few well-tested (Ref. 17, Ref. 19) modifications, such as production limiters for both k and ω, the use of S instead of Ω in the limiter for μ_T and a sharper cutoff for the cross-diffusion term.

It is also a low Reynolds number model, that is, it does not apply wall functions. A "low Reynolds number" refers to the region close to the wall where viscous effects dominate. The model equations are formulated in terms k and ω,

$$\begin{aligned}\rho\frac{\partial k}{\partial t}+\rho\mathbf{u}\cdot\nabla k &= P-\rho\beta_0^* k\omega+\nabla\cdot((\mu+\sigma_k\mu_T)\nabla k)\\ \rho\frac{\partial \omega}{\partial t}+\rho\mathbf{u}\cdot\nabla\omega &= \frac{\rho\gamma_\omega}{\mu_T}P-\rho\beta\omega^2+\nabla\cdot((\mu+\sigma_\omega\mu_T)\nabla\omega)+2(1-f_{v1})\frac{\rho\sigma_{\omega 2}}{\omega}\nabla\omega\cdot\nabla k\end{aligned} \tag{3-124}$$

where,

$$P = \min(P_k, 10\rho\beta_0^* k\omega) \tag{3-125}$$

and P_k is given in Equation 3-91. The turbulent viscosity is given by,

$$\mu_T = \frac{\rho a_1 k}{\max(a_1\omega, Sf_{v2})} \tag{3-126}$$

where S is the characteristic magnitude of the mean velocity gradients,

$$S = \sqrt{2S_{ij}S_{ij}} \tag{3-127}$$

The model constants are defined through interpolation of appropriate inner and outer values,

$$\phi = f_{v1}\phi_1 + (1 - f_{v1})\phi_2 \quad \text{for} \quad \phi = \beta, \gamma_\omega, \sigma_k, \sigma_\omega \tag{3-128}$$

The interpolation functions f_{v1} and f_{v2} are defined as

$$\begin{aligned} f_{v1} &= \tanh(\theta_1^4) \\ \theta_1 &= \min\left[\max\left(\frac{\sqrt{k}}{\beta_0^* \omega l_w}, \frac{500\mu}{\rho\omega l_w^2}\right), \frac{4\rho\sigma_{\omega 2} k}{CD_{k\omega} l_w^2}\right] \\ CD_{k\omega} &= \max\left(\frac{2\rho\sigma_{\omega 2}}{\omega}\nabla\omega \cdot \nabla k, 10^{-10}\right) \end{aligned} \tag{3-129}$$

and,

$$\begin{aligned} f_{v2} &= \tanh(\theta_2^2) \\ \theta_2 &= \max\left(\frac{2\sqrt{k}}{\beta_0^* \omega l_w}, \frac{500\mu}{\rho\omega l_w^2}\right) \end{aligned} \tag{3-130}$$

where l_w is the distance to the closest wall.

Realizability Constraints are applied to the SST model.

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the SST model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

The default model constants are given by,

$$\begin{aligned}\beta_1 &= 0.075, \quad \gamma_1 = 5/9, \quad \sigma_{k1} = 0.85, \quad \sigma_{\omega 1} = 0.5\\ \beta_2 &= 0.0828, \quad \gamma_2 = 0.44, \quad \sigma_{k2} = 1.0, \quad \sigma_{\omega 2} = 0.856\\ \beta_0^* &= 0.09, \quad a_1 = 0.31\end{aligned} \tag{3-131}$$

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

When **Wall Treatment** is set to **Automatic** the same type of formulation described for the k-ω model is applied at the boundary but with β_1 instead of β_0. See Automatic Wall Treatment for more details.

Low Reynolds Number

The SST model is low-Reynolds-number model, so the equations can be integrated all the way through the boundary layer to the wall, which allows for a no slip condition to be applied to the velocity, that is $\mathbf{u} = \mathbf{0}$.

Since all velocities must disappear on the wall, so must k. Hence, $k = 0$ on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_w \to 0} \omega = \frac{6\mu}{\rho \beta_1 l_w^2} \tag{3-132}$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-132 (using the variable ω_w, which only exists in those cells). Accurate solutions in the near-wall region require that the wall resolution in viscous units

$$\Delta_w^+ = \rho u_\tau h_w / \mu \sim 1 \tag{3-133}$$

where the resolution height is based on the distance between the first computational node inside the domain and the wall. u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \tag{3-134}$$

and is available as the postprocessing variable $u_{\tau w}$ (`u_tauWall`). Also, the boundary variable **Distance to cell center in viscous units**, l_c^+ (`lplus_cc`), is available to ensure that the mesh is fine enough. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell, thus $l_c^+ = 0.5\Delta_w^+$ and according to

Equation 3-133 l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

The postprocessing variable **Wall resolution in viscous units**, Δ_w^+ (`Delta_wPlus`), is available.

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the SST model.

FAR-FIELD BOUNDARY CONDITIONS

The SST model was originally developed for exterior aerodynamic simulations. The recommended far-field boundary conditions (Ref. 18) can be expressed as

$$\frac{10^{-5}U_\infty^2}{\mathrm{Re}_L} < k_\infty < \frac{0.1U_\infty^2}{\mathrm{Re}_L}$$
$$\frac{U_\infty}{L} < \omega_\infty < 10\frac{U_\infty}{L} \tag{3-135}$$

where L is the approximate length of the computational domain.

INITIAL VALUES

The SST model has the same default initial guess as the standard k-ω model (see Initial Values) but with $l_{\mathrm{mix}}^{\mathrm{lim}}$ replaced by l_{ref}.

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{\mathrm{ref}}$.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The SST model applies absolute scales of the same type as the k-ω model (see Scaling for Time-Dependent Simulations).

TRANSITION MODELING

The SST interface has an option to include a local, correlation-based transition model (Ref. 20). This enables modeling of the laminar portion of the boundary layer between the foremost stagnation point on a body and the point of transition. An additional transport equation for the intermittency, γ, is solved together with modified transport equations for k and ω. The transport equation for γ is given by,

$$\rho\frac{\partial\gamma}{\partial t}+\rho\mathbf{u}\cdot\nabla\gamma = P_\gamma - E_\gamma + \nabla\cdot\left(\left(\mu+\frac{\mu_T}{\sigma_\gamma}\right)\nabla\gamma\right) \tag{3-136}$$

where

$$P_\gamma = 100\rho S\gamma(1-\gamma)F_{\text{onset}}, \quad E_\gamma = c_{a2}\rho\Omega\gamma(c_{e2}\gamma-1)F_{\text{turb}} \tag{3-137}$$

The first two terms on the right hand side of the k-equation (Equation 3-124) are replaced by

$$\gamma\mu_T S\Omega + P^{\text{lim}} - \max(\gamma, 0.1)\rho\beta_0^*\omega k \tag{3-138}$$

where

$$P^{\text{lim}} = 5C_k\max(\gamma-0.2,0)(1-\gamma)F_{\text{on}}^{\text{lim}}\max(3C_{\text{SEP}}\mu-\mu_T, 0)S\Omega \tag{3-139}$$

The first term on the right hand side of the ω-equation (Equation 3-124) is replaced by

$$\gamma_\omega\rho\Omega^2 \tag{3-140}$$

The functions F_{turb} and $F_{\text{on}}^{\text{lim}}$ are given by

$$F_{\text{turb}} = e^{-\left(\frac{R_T}{2}\right)^4} \tag{3-141}$$

where

$$R_T = \frac{\rho k}{\omega\mu} \tag{3-142}$$

and

$$F_{\text{on}}^{\text{lim}} = \min\left(\max\left(\frac{R_V}{2.2\,\text{Re}_{\theta_c}^{\text{lim}}}-1,0\right), 3\right) \tag{3-143}$$

where

$$R_V = \frac{\rho l_w^2 S}{\mu} \tag{3-144}$$

and the constants are chosen as

$$\sigma_\gamma = 1, \quad c_{a2} = 0.06, \quad c_{e2} = 50, \quad C_k = 1.0, \quad C_{SEP} = 1.0, \quad \mathrm{Re}_{\theta_c}^{\lim} = 1100 \tag{3-145}$$

In addition, the function f_{v1} in Equation 3-129 is forced to be equal to one in the laminar portion of the boundary layer

$$f_{v1} = \max\left(\tanh(\theta_1^4), e^{-\left(\frac{R_y}{120}\right)^8}\right) \tag{3-146}$$

where

$$R_y = \frac{\rho l_w \sqrt{k}}{\mu} \tag{3-147}$$

The function predicting onset in Equation 3-137 is given by

$$F_{onset} = \max\left(\min\left(\frac{R_V}{2.2\mathrm{Re}_{\theta_c}}, 2\right) - \max\left(1 - \left(\frac{R_T}{3.5}\right)^3, 0\right), 0\right) \tag{3-148}$$

where the critical Reynolds number is taken as an empirical correlation depending on the turbulence intensity, Tu_L, and the limited pressure gradient parameter, $\lambda_{\theta,L}$, defined as

$$\mathrm{Tu}_L = \min\left(100\frac{\sqrt{2k/3}}{\omega l_w}, 100\right) \tag{3-149}$$

and

$$\lambda_{\theta,L} = \min\left(\max\left(7.57 \cdot 10^{-3}\frac{\rho l_w^2}{\mu}\frac{dU}{ds} + 0.0128, -1\right), 1\right) \tag{3-150}$$

where dU/ds is the velocity derivative in the streamwise direction. The empirical correlation function is given by

$$\mathrm{Re}_{\theta_c}(\mathrm{Tu}_L, \lambda_{\theta,L}) = C_{TU1} + C_{TU2}e^{-C_{TU3}\mathrm{Tu}_L F_{PG}(\lambda_{\theta,L})} \tag{3-151}$$

with

$$C_{TU1} = 100, \quad C_{TU2} = 1000, \quad C_{TU3} = 1 \tag{3-152}$$

$F_{PG}(\lambda_{\theta,L})$ is an empirical function given by

$$F_{\mathrm{PG}}(\lambda_{\theta,\mathrm{L}}) = \begin{cases} \min(1 + C_{\mathrm{PG1}}\lambda_{\theta,\mathrm{L}}, C_{\mathrm{PG1}}^{\lim}), & \text{for } \lambda_{\theta,\mathrm{L}} \geq 0 \\ \min(1 + C_{\mathrm{PG1}}\lambda_{\theta,\mathrm{L}} + & \\ \quad C_{\mathrm{PG3}}\min[\lambda_{\theta,\mathrm{L}} + 0.0681, 0], C_{\mathrm{PG2}}^{\lim}), & \text{for } \lambda_{\theta,\mathrm{L}} < 0 \end{cases} \quad (3\text{-}153)$$

where the constants

$$\begin{aligned} C_{\mathrm{PG1}} &= 14.68,\ C_{\mathrm{PG2}} = -7.34,\ C_{\mathrm{PG3}} = 0 \\ C_{\mathrm{PG1}}^{\lim} &= 1.5 \qquad C_{\mathrm{PG2}}^{\lim} = 3.0 \end{aligned} \quad (3\text{-}154)$$

are calibrated against Falkner–Skan profiles. Furthermore, the function $F_{\mathrm{PG}}(\lambda_{\theta,\mathrm{L}})$ is limited to positive values.

When the transition model is activated, only low-Reynolds-number wall treatment is available, and the mesh must be fine enough to resolve the laminar portion of the boundary layer. The boundary condition for w is also modified when using the transition model

$$\lim_{l_w \to 0} \omega = 10 \cdot \frac{6\mu}{\rho\beta_1 l_w^2} \quad (3\text{-}155)$$

In the *COMSOL Multiphysics Reference Manual:*

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The Low Reynolds Number k-ε Turbulence Model

When the accuracy provided by wall functions in the k-ε model is not enough, a so called *low Reynolds number* model can be used. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate.

Most low Reynolds number k-ε models adapt the turbulence transport equations by introducing damping functions. This module includes the AKN model (after the inventors Abe, Kondoh, and Nagano; Ref. 12). The AKN k-ε model for compressible flows reads (Ref. 8 and Ref. 12):

$$\rho\frac{\partial k}{\partial t}+\rho\mathbf{u}\cdot\nabla k=\nabla\cdot\left(\left(\mu+\frac{\mu_T}{\sigma_k}\right)\nabla k\right)+P_k-\rho\varepsilon$$
$$\rho\frac{\partial \varepsilon}{\partial t}+\rho\mathbf{u}\cdot\nabla \varepsilon=\nabla\cdot\left(\left(\mu+\frac{\mu_T}{\sigma_\varepsilon}\right)\nabla\varepsilon\right)+C_{\varepsilon 1}\frac{\varepsilon}{k}P_k-f_\varepsilon C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} \quad (3\text{-}156)$$

where

$$P_k=\mu_T\left(\nabla\mathbf{u}:(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}(\nabla\cdot\mathbf{u})^2\right)-\frac{2}{3}\rho k\nabla\cdot\mathbf{u}$$
$$\mu_T=\rho f_\mu C_\mu\frac{k^2}{\varepsilon}$$
$$f_\mu=(1-e^{-l^*/14})^2\cdot\left(1+\frac{5}{R_t^{3/4}}e^{-(R_t/200)^2}\right) \quad (3\text{-}157)$$
$$f_\varepsilon=(1-e^{-l^*/3.1})^2\cdot(1-0.3e^{-(R_t/6.5)^2})$$
$$l^*=(\rho u_\varepsilon l_w)/\mu\quad R_t=\rho k^2/(\mu\varepsilon)\quad u_\varepsilon=(\mu\varepsilon/\rho)^{1/4}$$

and

$$C_{\varepsilon 1}=1.5\quad C_{\varepsilon 2}=1.9\quad C_\mu=0.09\quad \sigma_k=1.4\quad \sigma_\varepsilon=1.4 \quad (3\text{-}158)$$

l_w is the distance to the closest wall.

Realizability Constraints are applied to the low Reynolds number k-ε model.

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the low Reynolds number k-ε model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. A formulation for ω-based methods was described by Menter and others in Ref. 9. The Low-Reynolds number model uses a similar formulation and defines

$$u_\tau^{\text{visc}} = \sqrt{\frac{\nu U_\parallel}{\delta_w}} \qquad u^{*,\log} = \sqrt[4]{C_\mu}\sqrt{k} \tag{3-159}$$

and

$$u^* = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u^{*,\log})^4} \tag{3-160}$$

δ_w is the distance to the closest wall. The boundary conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \mathbf{K} - (\mathbf{n} \cdot \mathbf{K} \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^+} \tag{3-161}$$

In Equation 3-161, $u^+ = U_\parallel / u_\tau$ with

$$u_\tau = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u_\tau^{\log})^4} \tag{3-162}$$

where in turn

$$u_\tau^{\log} = \frac{U_\parallel}{\frac{1}{\kappa_v}\log(\delta_w^+) + B} \tag{3-163}$$

Here, κ_v, is the von Kármán constant (default value 0.41), $U_\parallel$ is the velocity parallel to the wall, and B is a constant that by default is set to 5.2.

These expression can be combined with the lift-off concept shown in Figure 3-7 which gives $\delta_w = h_w/2$. The k-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all δ_w^+.

The conditions for the turbulent dissipation, ε, is given by the Wolfshtein model, which is commonly employed in two-layer k-ε implementations (Ref. 13):

$$\varepsilon = \frac{k^{3/2}}{l_\varepsilon}$$

$$l_\varepsilon = C_l \delta_w (1 - e^{-\mathrm{Re}_{\delta_w}/A_\varepsilon}) \qquad C_l = \kappa_v C_\mu^{-3} \S 4 \qquad (3\text{-}164)$$

$$A_\varepsilon = 2C_l \qquad \mathrm{Re}_y = \frac{\delta_w \sqrt{k}}{\nu}$$

The postprocessing variable for friction velocity $u_{\tau w}$ (`u_tauWall`) is based on the effective traction at the wall and is defined as

$$u_{\tau w} = \sqrt{u_\tau u^*}$$

while the postprocessing variable for the resulting wall resolution, Δ_w^+ (`Delta_wPlus`), is based on $u_{\tau w}$ and is defined as

$$\Delta_w^+ = \frac{u_{\tau w} \delta_w}{\nu}$$

Low Reynolds Number Wall Treatment

The damping terms in the equations for k and ε allow for a no slip condition to be applied to the velocity, that is $\mathbf{u} = \mathbf{0}$ which is the case when **Wall Treatment** is set to **Low Re**.

Since all velocities must disappear on the wall, so must k. Hence, $k = 0$ on the wall.

The correct wall boundary condition for ε is

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2 \qquad (3\text{-}165)$$

where n is the wall normal direction. This condition is however numerically very unstable. Therefore, ε is not solved for in the cells adjacent to a solid wall and instead the analytical relation

$$\varepsilon = 2\frac{\mu}{\rho}\frac{k}{l_w^2} \qquad (3\text{-}166)$$

is prescribed in those cells (using the variable ε_w, which only exists in those cells). Equation 3-166 can be derived as the first term in a series expansion of Equation 3-165.

For the expansion to be valid, and to obtain an accurate solution in the near-wall region, it is needed that the wall resolution in viscous units

$$\Delta_w^+ = \rho u_\tau h_w / \mu < 1 \tag{3-167}$$

where the resolution height is based on the distance between the first computational node inside the domain and the wall. u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \tag{3-168}$$

and is available as the postprocessing variable $u_{\tau w}$ (`u_tauWall`). Also, the boundary variable **Distance to cell center in viscous units**, l_c^+ (`lplus_cc`), is available to ensure that the mesh is fine enough. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell, thus $l_c^+ = 0.5\Delta_w^+$ and according to Equation 3-167 l_c^+ should be about 0.5. Observe that it is unlikely that a solution is obtained at all if

$$l_c^+ \gg 0.5$$

However, very small values of l_c^+ can reduce the convergence rate.

The postprocessing variable **Wall resolution in viscous units**, Δ_w^+ (`Delta_wPlus`), is available.

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the low-Reynolds number k-ε model.

INITIAL VALUES

The low-Reynolds number k-ε model has the same default initial guess as the standard k-ε model (see Initial Values) but with l_{mix}^{lim} replaced by l_{ref}.

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

In some cases, especially for stationary solutions, a fast way to convergence is to first solve the model using the ordinary k-ε model and then to use that solution as an initial guess for the low-Reynolds number k-ε model. The procedure is then as follows:

1. Solve the model using the k-ε model.
2. Switch to the low-Reynolds number k-ε model.
3. Add a new **Stationary with Initialization** study.

4 In the **Wall Distance Initialization** study step, set **Values of variables not solved for** to **Solution** from the first study. This is to propagate the solution from the first study down to the second step in the new study.

5 Solve the new study.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The low-Reynolds number k-ε model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations).

In the *COMSOL Multiphysics Reference Manual:*

- The Wall Distance Interface

Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The Spalart–Allmaras Turbulence Model

The *Spalart–Allmaras turbulence model* is a one-equation turbulence model designed mainly for aerodynamic applications. It is a low Reynolds number model, that is, it does not utilize wall functions. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate.

The model gives satisfactory results for many engineering applications, in particular for airfoil and turbine blade applications for which it is calibrated. It is however not appropriate for applications involving jet-like free shear regions. It also has some unphysical properties. For example, it predicts zero decay rate for the eddy viscosity in a uniform free-stream (Ref. 1).

Compared to the low Reynolds number k-ε model, the Spalart–Allmaras model is generally considered more robust and is often used as a way to obtain an initial solution for more advanced models. It can give reasonable results on relatively coarse meshes for which the low Reynolds number k-ε model does not converge or even diverges.

This module includes the standard version of the Spalart–Allmaras model without the trip term (see Ref. 1 and Ref. 15). The model solves for the undamped turbulent kinematic viscosity, ν :

$$\frac{\partial \tilde{\nu}}{\partial t} + \mathbf{u} \cdot \nabla \tilde{\nu} = c_{b1} S \tilde{\nu} - c_{w1} f_w \left(\frac{\tilde{\nu}}{l_w}\right)^2 + \frac{1}{\sigma} \nabla \cdot ((\nu + \tilde{\nu}) \nabla \tilde{\nu}) + \frac{c_{b2}}{\sigma} \nabla \tilde{\nu} \cdot \nabla \tilde{\nu} \qquad (3\text{-}169)$$

The model includes the following auxiliary variables

$$c_{w1} = \frac{c_{b1}}{\kappa_v^2} + \frac{1 + c_{b2}}{\sigma}, \quad \chi = \frac{\tilde{\nu}}{\nu}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}$$

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_w = g\left(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6}\right)^{1/6}, \quad g = r + c_{w2}(r^6 - r)$$

$$r = \min\left(\frac{\tilde{\nu}}{\tilde{S}\kappa_v^2 l_w^2}, 10\right), \quad \tilde{S} = \max\left(\Omega + C_{Rot}\min(0, S - \Omega) + \frac{\tilde{\nu}}{\kappa_v^2 l_w^2} f_{v2}, 0.3\Omega\right)$$

$$S = \sqrt{2S_{ij}S_{ij}} \qquad \Omega = \sqrt{2\Omega_{ij}\Omega_{ij}}$$

where

$$S_{ij} = 0.5(\nabla \mathbf{u} + \nabla \mathbf{u}^T) \qquad \Omega_{ij} = 0.5(\nabla \mathbf{u} - \nabla \mathbf{u}^T)$$

are the mean strain rate and mean rotation rate tensors, l_w, is the distance to the closest wall and $\nu = \mu/\rho$ is the kinematic viscosity. The turbulent viscosity is calculated by

$$\mu_T = \rho \nu f_{v1}$$

The default values for the modeling parameters are:

$$c_{b1} = 0.1355 \quad c_{b2} = 0.622 \quad c_{v1} = 7.1 \quad \sigma = 2/3$$
$$c_{w2} = 0.3 \quad c_{w3} = 2 \quad \kappa_v = 0.41 \quad C_{Rot} = 2.0$$

The implementation of the production term $\tilde{S}$ includes the rotation correction suggested in Ref. 15. See also Ref. 16. The terms r and $\tilde{S}$ are furthermore regularized according to Ref. 15.

Pseudo Time Stepping for Turbulent Flow Models is by default applied to the stationary form of the Spalart–Allmaras model.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

For the Spalart–Allmaras turbulence model, the following relation is valid from the wall all the way through the log layer (Ref. 26):

$$\tilde{\nu} = \kappa_v \delta_w u_\tau \quad \Leftrightarrow \quad \tilde{\nu}^+ = \frac{\tilde{\nu}}{\nu} = \frac{\kappa_v \delta_w u_\tau}{\nu} = \kappa_v \delta_w^+ \tag{3-170}$$

$\delta_w{}^+$ from Equation 3-170 can be used in Equation 3-112 to calculate $u_\tau{}^{\log}$ which in turn gives u_τ through Equation 3-114. With u_τ, the boundary condition for ν is given by $\tilde{\nu} = \kappa_v \delta_w u_\tau$.

These relations are applied to the lift-off concept shown in Figure 3-7, which gives $\delta_w = h_w/2$. The boundary conditions for the momentum equations are a no-penetration condition, $\mathbf{u}\cdot\mathbf{n} = 0$ and the traction condition given by Equation 3-115.

The postprocessing variable for friction velocity is available as $u_{\tau w}$ (`u_tauWall`) while the postprocessing variable for the resulting wall resolution Δ_w^+ (`Delta_wPlus`) is based on $u_{\tau w}$ and is defined as

$$\Delta_w^+ = \frac{u_{\tau w}\delta_w}{\nu}$$

Low Reynolds Number Wall Treatment

The Spalart–Allmaras model is consistent with a no-slip boundary condition; that is, $\mathbf{u} = 0$. Since there can be no fluctuations on the wall, the boundary condition for ν is $\nu = 0$.

The Spalart–Allmaras model can be considered to be well resolved at a wall if $l_c^+ < 0.5$. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell and can be evaluated as the boundary variable **Distance to cell center in viscous units**, `lplus_cc`. See Low Reynolds Number Wall Treatment for the boundary condition details and definition of the postprocessing variables $u_{\tau w}$ (`u_tauWall`) and Δ_w^+ (`Delta_wPlus`).

INITIAL VALUES

The default initial values for the Spalart–Allmaras version of the physics interface are:

$$\mathbf{u} = 0$$
$$p = 0$$
$$\tilde{\nu} = \frac{\mu}{\rho}$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The Spalart–Allmaras model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations) except that the scale for ν is given directly by the ν_{scale} parameter available in the advanced section of the physics interface node. The default value for ν_{scale} is $5 \cdot 10^{-6}$ m^2/s.

The v2-f Turbulence Model

For the v2-f model, the turbulent viscosity is based on the velocity fluctuations, $\overline{v^2}$, normal to the streamlines. This makes it possible to model turbulence anisotropy, and to separate between low-Reynolds number effects and wall blockage. Nonlocal effects of the pressure fluctuations on the turbulent fields are included by applying elliptic relaxation to the pressure strain term (Ref. 27, Ref. 28). The formulation implemented in COMSOL Multiphysics, solves for the normalized velocity fluctuations,

$$\zeta = \frac{\overline{v^2}}{k} \tag{3-171}$$

and an elliptic blending function, α, which is used to combine near-wall effects with those in the far-field. The complete model for compressible flow reads,

$$\begin{aligned}
\rho\frac{\partial k}{\partial t} + \rho\mathbf{u}\cdot\nabla k &= \nabla\cdot\left(\left(\mu + \frac{\mu_T}{\sigma_{kv2f}}\right)\nabla k\right) + P_k - \rho\varepsilon \\
\rho\frac{\partial \varepsilon}{\partial t} + \rho\mathbf{u}\cdot\nabla \varepsilon &= \nabla\cdot\left(\left(\mu + \frac{\mu_T}{\sigma_{\varepsilon v2f}}\right)\nabla \varepsilon\right) + \frac{1}{\tau}(C'_{\varepsilon 1}P_k - C'_{\varepsilon 2}\rho\varepsilon) \\
\rho\frac{\partial \zeta}{\partial t} + \rho\mathbf{u}\cdot\nabla \zeta &= \nabla\cdot\left(\left(\mu + \frac{\mu_T}{\sigma_{\zeta v2f}}\right)\nabla \zeta\right) + \frac{2}{k}\left(\alpha^3\mu + \frac{\mu_T}{\sigma_{kv2f}}\right)\nabla k\cdot\nabla\zeta \\
&\quad - \frac{\zeta}{k}P_k + \alpha^3 f_h + (1-\alpha^3)f_w \\
\nabla^2\alpha &= \frac{\alpha - 1}{L^2}
\end{aligned} \tag{3-172}$$

where

$$P_k = \mu_T\left(\nabla\mathbf{u}:(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}(\nabla\cdot\mathbf{u})^2\right)-\frac{2}{3}\rho k\nabla\cdot\mathbf{u}$$
$$\mu_T = \rho C_{\mu v2f} k\zeta\tau$$
$$f_h = -\frac{\rho}{\tau}\left(C_1 - 1 + C_2\frac{P_k}{\rho\varepsilon}\right)\left(\zeta-\frac{2}{3}\right) \qquad (3\text{-}173)$$
$$f_w = -\rho\frac{\zeta}{k}\varepsilon$$
$$L = C_L\max\left[\frac{k^{3/2}}{\varepsilon}, C_\eta\left(\frac{\nu^3}{\varepsilon}\right)^{1/4}\right] \quad \tau = \max\left[\frac{k}{\varepsilon}, C_\tau\sqrt{\frac{\nu}{\varepsilon}}\right]$$

where $\nu = \mu/\rho$. The modified coefficients in the ε-equation are given by

$$C'_{\varepsilon 1} = C_{\varepsilon 1 v2f}\left(1+A_1(1-\alpha^3)\frac{1}{\sqrt{\zeta}}\right)$$
$$C'_{\varepsilon 2} = C_{\varepsilon 2 v2f}+\alpha^3(1-C_{\varepsilon 2 v2f})\tanh\left(\left|\frac{\mu_T\nabla^2 k}{\rho\varepsilon}\right|^{3/2}\right) \qquad (3\text{-}174)$$

with the default turbulence parameters

$$C_{\varepsilon 1 v2f} = 1.44 \quad C_{\varepsilon 2 v2f} = 1.83 \quad C_{\mu v2f} = 0.22 \quad \sigma_{kv2f} = \sigma_{\zeta v2f} = 1$$
$$\sigma_\varepsilon = 1.22 \quad C_1 = 1.7 \quad C_2 = 1.2 \quad C_\eta = 86 \qquad (3\text{-}175)$$
$$C_\tau = 6 \quad A_1 = 0.04$$

Realizability Constraints are applied to the turbulent viscosity.

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the v2-f model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this

purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. A formulation for ω-based methods was described by Menter and others in Ref. 9. The v2-f model uses a similar formulation and defines

$$u_\tau^{\text{visc}} = \sqrt{\frac{\nu U_\parallel}{\delta_w}} \qquad u^{*,\log} = \sqrt[4]{C_{\mu v2f}\zeta}\sqrt{k} \tag{3-176}$$

and

$$u^* = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u^{*,\log})^4} \tag{3-177}$$

δ_w is the distance to the closest wall. The boundary conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \mathbf{K} - (\mathbf{n} \cdot \mathbf{K} \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^+} \tag{3-178}$$

In Equation 3-178, $u^+ = U_\parallel / u_\tau$ with

$$u_\tau = \sqrt[4]{(u_\tau^{\text{visc}})^4 + (u_\tau^{\log})^4} \tag{3-179}$$

where in turn

$$u_\tau^{\log} = \frac{U_\parallel}{\frac{1}{\kappa_v}\log(\delta_w^+) + B} \tag{3-180}$$

Here, κ_v, is the von Kármán constant (default value 0.41), $U_\parallel$ is the velocity parallel to the wall, and B is a constant that by default is set to 5.2.

These expression can be combined with the lift-off concept shown in Figure 3-7 which gives $\delta_w = h_w/2$. The k-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all δ_w^+.

The conditions for the turbulent dissipation rate, ε, is similar to that in the Wolfshtein model which is commonly employed in two-layer k-ε implementations (Ref. 13):

$$\begin{aligned} \varepsilon &= \frac{(C_{\mu v2f}\zeta_0)^{3/4}k^{3/2}}{l_\varepsilon} \\ l_\varepsilon &= L\left(1 - e^{-\sqrt{\mathrm{Re}_L}(\delta_w/L)}\right)^2 \\ \mathrm{Re}_y &= \frac{(C_{\mu v2f}\zeta_0)^{3/4}\sqrt{k}L}{2\nu} \end{aligned} \tag{3-181}$$

where

$$\zeta_0 = \frac{2}{3}\left(1 - \frac{1}{C_1 + C_2}\right) \tag{3-182}$$

The boundary conditions applied on ζ and α are given by

$$\zeta = \zeta_0 \frac{\delta_w^2}{\delta_w^2 + L^2} \qquad \alpha = 1 - e^{-\delta_w/L} \tag{3-183}$$

The postprocessing variable for friction velocity $u_{\tau w}$ (`u_tauWall`) is based on the effective traction at the wall and is defined as

$$u_{\tau w} = \sqrt{u_\tau u^*}$$

while the postprocessing variable for the resulting wall resolution, Δ_w^+ (`Delta_wPlus`), is based on $u_{\tau w}$ (`u_tauWall`) and is defined as

$$\Delta_w^+ = \frac{u_{\tau w}\delta_w}{\nu}$$

Low Reynolds Number Wall Treatment

The no slip condition, that is $\mathbf{u} = \mathbf{0}$ is applied when **Wall Treatment** is set to **Low Re**.

Since all velocities must disappear on the wall, so must k and ζ (since $k \sim y^2$ and $\overline{v^2} \sim y^4$). Hence, $k = 0$ and $\zeta = 0$ on the wall. By definition, $\alpha = 0$ on the wall.

The correct wall boundary condition for ε is

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2 \tag{3-184}$$

where n is the wall normal direction. This condition is however numerically very unstable. Therefore, ε is not solved for in the cells adjacent to a solid wall and instead the analytical relation

$$\varepsilon = 2\frac{\mu}{\rho}\frac{k}{l_w^2} \tag{3-185}$$

is prescribed in those cells (using the variable ε_w, which only exists in those cells). Equation 3-185 can be derived as the first term in a series expansion of Equation 3-184.

For the expansion to be valid, it is required that

$$l_c^+ < 0.5$$

l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell. The boundary variable **Distance to cell center in viscous units**, `lplus_cc`, is available to ensure that the mesh is fine enough. Observe that it is unlikely that a solution is obtained at all if

$$l_c^+ \gg 0.5$$

See Low Reynolds Number Wall Treatment for the boundary condition details and definition of the postprocessing variables $u_{\tau w}$ (`u_tauWall`) and Δ_w^+ (`Delta_wPlus`).

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the v2-f model.

INITIAL VALUES

The v2-f model has the same default initial guess as the standard k-ε model (see Initial Values) but with l_{mix}^{lim} replaced by l_{ref}. The default initial values for ζ and α are 2/3 and 1 respectively.

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

In some cases, especially for stationary solutions, a fast way to convergence is to first solve the model using the ordinary k-ε model and then to use that solution as an initial guess for the v2-f model. The procedure is then as follows:

1. Solve the model using the k-ε model.
2. Switch to the v2-f model.
3. Add a new **Stationary with Initialization** study.
4. In the **Wall Distance Initialization** study step, set **Values of variables not solved for** to **Solution** from the first study. This is to propagate the solution from the first study down to the second step in the new study.
5. Solve the new study.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The v2-f model applies absolute scales of the same type as the k-ε model (see Scaling for Time-Dependent Simulations).

In the *COMSOL Multiphysics Reference Manual:*

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The Wilcox R-ω Turbulence Model

The Wilcox R-ω model belongs to RANS-RSM type of turbulence models and, hence, does not assume a particular form of $\mathbf{R} = \overline{\mathbf{u}' \otimes \mathbf{u}'}$ (the kinematic Reynolds stress tensor). It solves the transport equation for $\mathbf{R}$ instead, complemented by the transport equation for the turbulence specific dissipation rate ω, which allows to capture the evolution of turbulence structure properly Ref. 32. This leads to more accurate prediction of separation, transient phenomena, effects of swirl and curvature. Moreover, correct description of secondary flows is achieved, which eddy-viscosity based models are intrinsically incapable of.

In COMSOL Multiphysics the equations for the Wilcox R-ω model are implemented in fully compressible form and are compatible with most Multiphysics Couplings available for a RANS-EVM.

The set of Wilcox R-ω model parameters with their default values is

$$\alpha = \frac{13}{25} \quad \sigma^* = \frac{1}{2} \quad \sigma_\omega = \frac{1}{2} \quad \beta_{0W} = 0.0708 \quad \beta_0^* = \frac{9}{100}$$
$$c_1^{PS} = 1.8 \quad c_2^{PS} = \frac{10}{19} \tag{3-186}$$

The expressions for the turbulence kinetic energy, turbulence viscosity, turbulence dissipation rate, turbulence time-scale, and turbulence frequency-scale are

$$k = \frac{R_{ii}}{2} \quad \mu_T = \rho\frac{k}{\omega} \quad \varepsilon = \beta_0^*\omega k \quad \tau_T = \frac{k}{\varepsilon} \quad \gamma_T = \frac{\varepsilon}{k} \tag{3-187}$$

The turbulence anisotropy tensor is defined as

$$a_{ij} = \frac{R_{ij}}{k} - \frac{2}{3}\delta_{ij} \tag{3-188}$$

The **R**-equation is stated as

$$\rho\frac{\partial R_{ij}}{\partial t} + \rho U_k\frac{\partial R_{ij}}{\partial x_k} = P_{ij} + \Pi_{ij} - \rho\varepsilon_{ij} + D_{ij} \tag{3-189}$$

This is a symmetric tensor equation that consists of six scalar equations. The production term P_{ij} (as well as P - production term of k) has explicit form

$$P_{ij} = -\rho\left(R_{ik}\frac{\partial U_j}{\partial x_k} + R_{jk}\frac{\partial U_i}{\partial x_k}\right) \qquad P = -\rho R_{ij}\frac{\partial U_i}{\partial x_j} \tag{3-190}$$

Of primary importance for a Reynolds Stress Model is the modeling of the pressure–strain correlation Π_{ij}:

$$\begin{aligned}\Pi_{ij} = &-\rho\, c_1^{PS}\varepsilon a_{ij} + \rho\frac{4}{5}k S_{ij} + \\ &\rho\frac{9\cdot c_2^{PS} + 6}{11}k\left(a_{ik}S_{kj} + S_{ik}a_{kj} - \frac{2}{3}a_{kl}S_{kl}\delta_{ij}\right) + \\ &\rho\frac{10 - 7\cdot c_2^{PS}}{11}k\left(\Omega_{ik}a_{kj} - a_{ik}\Omega_{kj}\right)\end{aligned} \tag{3-191}$$

which is responsible for the redistribution of the turbulence kinetic energy among the components of **R**. For Wilcox R-ω it involves two model parameters.

The turbulent diffusion **D** and turbulent dissipation ε_{ij} of **R** are modeled as

$$D_{ij} = \frac{\partial}{\partial x_k}\left((\mu + \sigma^* \mu_T)\frac{\partial R_{ij}}{\partial x_k}\right) \qquad \varepsilon_{ij} = \frac{2}{3}\varepsilon\delta_{ij} \tag{3-192}$$

The ω-equation is stated as

$$\rho\frac{\partial \omega}{\partial t} + \rho U_k \frac{\partial \omega}{\partial x_k} = \alpha\frac{\omega}{k}P - \rho\beta_W\omega^2 + \nabla\cdot((\mu + \sigma_\omega\mu_T)\nabla\omega) + \frac{\rho\sigma_d}{\omega}\nabla\omega\cdot\nabla k \tag{3-193}$$

where

$$\beta_W = \beta_{0W}\frac{1+85\chi_\omega}{1+100\chi_\omega} \qquad \chi_\omega = \left|\frac{\Omega_{ij}\Omega_{jk}S_{ki}}{(\beta_0^*\omega)^3}\right| \qquad \sigma_d = \frac{1}{8}(\nabla\omega\cdot\nabla k > 0) \tag{3-194}$$

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the Wilcox R-ω model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

When there is no Moving Mesh, the equation for the wall distance variable can be solved once only. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITIONS

Low Reynolds Number Wall Treatment

The Wilcox R-ω turbulence model can be integrated all the way down to the wall and is consistent with the no-slip condition $\mathbf{u} = 0$. Since fluctuations of velocity must disappear on the wall, so must $\mathbf{R}$. Hence, $\mathbf{R} = \mathbf{0}$ on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_w \to 0}\omega = \frac{6\mu}{\rho\beta_{0W}l_w^2} \tag{3-195}$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-195 (using the variable ω_w, which only exists in those cells). Accurate solutions in the near-wall region require that the wall resolution in viscous units

$$\Delta_w^+ = \rho u_\tau h_w / \mu \sim 1 \tag{3-196}$$

where the resolution height is based on the distance between the first computational node inside the domain and the wall. u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \tag{3-197}$$

and is available as the postprocessing variable $u_{\tau w}$ (`u_tauWall`). Also, the boundary variable **Distance to cell center in viscous units**, l_c^+ (`lplus_cc`), is available to ensure that the mesh is fine enough. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell, thus $l_c^+ = 0.5\Delta_w^+$ and according to Equation 3-196 l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate. Also notice that it is unlikely that a solution is obtained at all if

$$l_c^+ \gg 0.5$$

Since the ω_w variable requires the wall distance, a wall distance equation must be solved prior to solving the Wilcox R-ω model.

The postprocessing variable **Wall resolution in viscous units**, Δ_w^+ (`Delta_wPlus`), is available.

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the Wilcox R-ω model.

INITIAL VALUES

The Wilcox R-ω model essentially has the same default initial guess as the SST model, but for the Reynolds stress tensor instead of k:

$$\mathbf{u} = 0$$
$$p = 0$$
$$k_{\text{init}} = \left(\frac{10 \cdot \mu}{\rho(0.1 \cdot l_{\text{ref}})}\right)^2$$
$$\omega_{\text{init}} = \frac{\sqrt{k_{\text{init}}}}{0.1 \cdot l_{\text{ref}}}$$
$$R_{ij} = \frac{2}{3} k_{\text{init}} \delta_{ij}$$

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{\text{ref}}$.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The Wilcox R-ω model applies absolute scales of the same type as the SST model, namely

$$k_{\text{scale}} = (0.1 U_{\text{scale}})^2$$
$$R_{\text{scale}} = k_{\text{scale}}$$
$$\omega_{\text{scale}} = \frac{\sqrt{k_{\text{scale}}}}{L_{\text{fact}} \cdot l_{\text{bb, min}}}$$

In the *COMSOL Multiphysics Reference Manual:*

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The SSG-LRR Turbulence Model

The SSG-LRR model belongs to RANS-RSM type of turbulence models and, hence, does not assume a particular form of $\mathbf{R} = \overline{\mathbf{u}' \otimes \mathbf{u}'}$ (the kinematic Reynolds stress tensor). It solves the transport equation for $\mathbf{R}$ instead, complemented by the transport equation for the turbulence specific dissipation rate ω, which allows to capture the evolution of turbulence structure properly Ref. 33. This leads to more accurate prediction of separation, transient phenomena, effects of swirl and curvature. Moreover, correct description of secondary flows is achieved, which eddy-viscosity based models are intrinsically incapable of.

In COMSOL Multiphysics the equations for the SSG-LRR model are implemented in fully compressible form and are compatible with most Multiphysics Couplings available for a RANS-EVM.

The set of SSG-LRR model parameters with their default values is

$$\begin{array}{cccc} \alpha_\omega^{(\omega)} = 0.5556 & \alpha_\omega^{(\varepsilon)} = 0.44 & \beta_\omega^{(\omega)} = 0.075 & \beta_\omega^{(\varepsilon)} = 0.0828 \\ \sigma_\omega^{(\omega)} = 0.5 & \sigma_\omega^{(\varepsilon)} = 0.856 & \sigma_d^{(\omega)} = 0 & \sigma_d^{(\varepsilon)} = 1.712 \\ c_1^{\mathrm{PS},(\omega)} = 1.8 & c_1^{\mathrm{PS},(\varepsilon)} = 1.7 & c_1^{*,\mathrm{PS},(\omega)} = 0 & c_1^{*,\mathrm{PS},(\varepsilon)} = 0.9 \\ c_2^{\mathrm{PS},(\omega)} = 0 & c_2^{\mathrm{PS},(\varepsilon)} = 1.05 & & \\ c_3^{\mathrm{PS}} = 0.8 & & c_3^{*,\mathrm{PS},(\omega)} = 0 & c_3^{*,\mathrm{PS},(\varepsilon)} = 0.65 \\ c_4^{\mathrm{PS},(\omega)} = 0.971 & c_4^{\mathrm{PS},(\varepsilon)} = 0.625 & c_5^{\mathrm{PS},(\omega)} = 0.578 & c_5^{\mathrm{PS},(\varepsilon)} = 0.2 \\ C_\mu = 0.09 & & D^{(\omega)} = 0.0675 & D^{(\varepsilon)} = 0.22 \end{array} \quad (3\text{-}198)$$

Notice that

$$D^{(\omega)} = 0.75 \cdot C_\mu \quad c_4^{\mathrm{PS},(\omega)} = \frac{9 \cdot c_2^{\mathrm{PS,LRR}} + 6}{11} \quad c_5^{\mathrm{PS},(\omega)} = \frac{10 - 7 \cdot c_2^{\mathrm{PS,LRR}}}{11}$$

where the original Launder–Reece–Rodi expressions for the pressure-strain coefficients are stated using $c_2^{\mathrm{PS,LRR}} = 0.52$.

The expressions for the turbulence kinetic energy, turbulence viscosity, turbulence dissipation rate, turbulence time-scale, and turbulence frequency-scale are

$$k = \frac{R_{ii}}{2} \quad \mu_\mathrm{T} = \rho\frac{k}{\omega} \quad \varepsilon = C_\mu \omega k \quad \tau_\mathrm{T} = \frac{k}{\varepsilon} \quad \gamma_\mathrm{T} = \frac{\varepsilon}{k} \quad (3\text{-}199)$$

The turbulence anisotropy tensor is defined as

$$a_{ij} = \frac{R_{ij}}{k} - \frac{2}{3}\delta_{ij} \quad (3\text{-}200)$$

Similar to The SST Turbulence Model the model parameters are blended between ω-based and ε-based approaches as

$$\phi = F_1\phi^{(\omega)} + (1 - F_1)\phi^{(\varepsilon)}$$

$$\text{for } \phi = \alpha_\omega, \beta_\omega, \sigma_\omega, \sigma_d, c_1^{\mathrm{PS}}, c_1^{*,\mathrm{PS}}, c_2^{\mathrm{PS}}, c_3^{*,\mathrm{PS}}, c_4^{\mathrm{PS}}, c_5^{\mathrm{PS}}, D$$

The interpolation function F_1 is defined as

$$F_1 = \tanh(\theta_1^4)$$
$$\theta_1 = \min\left[\max\left(\frac{\sqrt{k}}{C_\mu \omega l_w}, \frac{500\mu}{\rho\omega l_w^2}\right), \frac{4\rho\sigma_\omega^{(\varepsilon)}k}{CD_1 l_w^2}\right] \tag{3-201}$$
$$CD_1 = \max\left(\frac{\sigma_d^{(\varepsilon)}}{\omega}\nabla\omega\cdot\nabla k, 10^{-20}\right)$$

where l_w is the distance to the closest wall.

Notice that c_3^{PS} avoids blending since its value follows from the rapid distortion theory.

The **R**-equation is stated as

$$\rho\frac{\partial R_{ij}}{\partial t} + \rho U_k \frac{\partial R_{ij}}{\partial x_k} = P_{ij} + \Pi_{ij} - \rho\varepsilon_{ij} + D_{ij} \tag{3-202}$$

This is a symmetric tensor equation that consists of six scalar equations. The production term P_{ij} (as well as P - production term of k) has explicit form,

$$P_{ij} = -\rho\left(R_{ik}\frac{\partial U_j}{\partial x_k} + R_{jk}\frac{\partial U_i}{\partial x_k}\right) \qquad P = -\rho R_{ij}\frac{\partial U_i}{\partial x_j} \tag{3-203}$$

Of primary importance for a Reynolds Stress Model is the modeling of the pressure–strain correlation Π_{ij}:

$$\begin{aligned}\Pi_{ij} = &-\rho(c_1^{PS}\varepsilon + c_1^{*,PS}P)a_{ij} + \rho c_2^{PS}\varepsilon\left(a_{ik}a_{kj} - \frac{1}{3}a_{kl}a_{kl}\delta_{ij}\right) + \\ &\rho(c_3^{PS} - c_3^{*,PS}\sqrt{a_{kl}a_{kl}})kS_{ij} + \\ &\rho c_4^{PS}k\left(a_{ik}S_{kj} + S_{ik}a_{kj} - \frac{2}{3}a_{kl}S_{kl}\delta_{ij}\right) + \\ &\rho c_5^{PS}k(\Omega_{ik}a_{kj} - a_{ik}\Omega_{kj})\end{aligned} \tag{3-204}$$

which is responsible for the redistribution of the turbulence kinetic energy among the components of **R**. For SSG-LRR it involves seven model parameters (after the blending is performed).

The turbulent diffusion **D** is modeled as a "simple diffusion"and turbulent dissipation ε_{ij} of **R** is modeled as isotropic

$$D_{ij} = \frac{\partial}{\partial x_k}\left((\mu + \sigma^* \mu_T)\frac{\partial R_{ij}}{\partial x_k}\right) \qquad \sigma^* = \frac{2}{3}\frac{D}{C_\mu} \qquad \varepsilon_{ij} = \frac{2}{3}\varepsilon\delta_{ij} \quad (3\text{-}205)$$

The ω-equation is stated as

$$\rho\frac{\partial \omega}{\partial t} + \rho U_k \frac{\partial \omega}{\partial x_k} = \alpha_\omega \frac{\omega}{k} P - \rho\beta_\omega \omega^2 + \nabla\cdot((\mu + \sigma_\omega \mu_T)\nabla\omega) + \frac{\rho\sigma_d}{\omega}\max(\nabla\omega\cdot\nabla k, 0) \quad (3\text{-}206)$$

WALL DISTANCE

The wall distance variable, l_w, is provided by a mathematical Wall Distance interface that is included when using the SSG-LRR model. The solution to the wall distance equation is controlled using the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

When there is no Moving Mesh, the equation for the wall distance variable can be solved once only. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITIONS

Low Reynolds Number Wall Treatment

The SSG-LRR turbulence model can be integrated all the way down to the wall and is consistent with the no-slip condition $\mathbf{u} = 0$. Since fluctuations of velocity must disappear on the wall, so must **R**. Hence, $\mathbf{R} = \mathbf{0}$ on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_w \to 0} \omega = \frac{6\mu}{\rho\beta_\omega^{(\omega)} l_w^2} \quad (3\text{-}207)$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-195 (using the variable ω_w, which

only exists in those cells). Accurate solutions in the near-wall region require that the wall resolution in viscous units

$$\Delta_w^+ = \rho u_\tau h_w / \mu \sim 1 \tag{3-208}$$

where the resolution height is based on the distance between the first computational node inside the domain and the wall. u_τ is the friction velocity which is calculated from the wall shear-stress τ_w,

$$u_\tau = \sqrt{\tau_w / \rho} \tag{3-209}$$

and is available as the postprocessing variable $u_{\tau w}$ (`u_tauWall`). Also, the boundary variable **Distance to cell center in viscous units**, l_c^+ (`lplus_cc`), is available to ensure that the mesh is fine enough. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell, thus $l_c^+ = 0.5\Delta_w^+$ and according to Equation 3-196 l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate. Also notice that it is unlikely that a solution is obtained at all if

$$l_c^+ \gg 0.5$$

Since the ω_w variable requires the wall distance, a wall distance equation must be solved prior to solving the SSG-LRR model.

The postprocessing variable **Wall resolution in viscous units**, Δ_w^+ (`Delta_wPlus`), is available.

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, L_T, and the turbulence intensity, I_T, apply also to the SSG-LRR model.

INITIAL VALUES

The SSG-LRR model essentially has the same default initial guess as the SST model, but for the Reynolds stress tensor instead of k:

$$\mathbf{u} = 0$$
$$p = 0$$
$$k_{\text{init}} = \left(\frac{10 \cdot \mu}{\rho(0.1 \cdot l_{\text{ref}})}\right)^2$$
$$\omega_{\text{init}} = \frac{\sqrt{k_{\text{init}}}}{0.1 \cdot l_{\text{ref}}}$$
$$R_{ij} = \frac{2}{3} k_{\text{init}} \delta_{ij}$$

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{\text{ref}}$.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The Wilcox R-ω model applies absolute scales of the same type as the SST model, namely

$$k_{\text{scale}} = (0.1 U_{\text{scale}})^2$$
$$R_{\text{scale}} = k_{\text{scale}}$$
$$\omega_{\text{scale}} = \frac{\sqrt{k_{\text{scale}}}}{L_{\text{fact}} \cdot l_{\text{bb, min}}}$$

In the *COMSOL Multiphysics Reference Manual*:

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

Theory for Turbulence in Porous Media

Since **Darcian flow** is not compatible with the character of a turbulent flow, only **Non-Darcian flow** is available in **Porous Medium** domains as a **Flow model** option when a two-equation turbulence model is activated. The turbulence equations are fully active in a **Porous Medium** and are modified according to the theory below. Currently, the algebraic turbulence models do not change the formulation of the momentum equation in porous domains and the Spalart–Allmaras model prohibits them.

AVERAGING IN POROUS MEDIA

A detailed description of turbulence in porous media can, in principle, be achieved by employing common turbulence modeling in the corresponding complex geometries. However, heavy computations would be needed when a characteristic size of the porous matrix cavities, or pores, is much smaller than the geometry dimensions. A characteristic size of the pores, the porous length scale, is given by $l_{\text{pore}} = \sqrt{\kappa/\varepsilon_p}$, where κ and ε_p are the medium's permeability and porosity, respectively. For this reason, a simplified framework for turbulence modeling in porous media has been developed. It is based on taking the turbulence equations in the interstitial space and averaging them over the whole combined volume of fluid and porous matrix (Ref. 30), a so-called *representative volume element* (RVE). In this framework, detailed information about the gradients of velocity and other quantities on the l_{pore}-scale is not available, but its influence is modeled by introducing extra terms that depend on the RVE-smoothed quantities.

For example, the averaging (or RVE-smoothing) rule for the mean velocity is

$$\mathbf{u} = \varepsilon_p \mathbf{u}^i \text{ where } \mathbf{u}^i = \frac{1}{\Delta V_f}\int_{\Delta V_f} \overline{\mathbf{u}^{\text{micro}}}\, dV, \quad \mathbf{u} = \frac{1}{\Delta V}\int_{\Delta V_f} \overline{\mathbf{u}^{\text{micro}}}\, dV \tag{3-210}$$

Here $\overline{\mathbf{u}^{\text{micro}}}$ is the Reynolds-averaged microscopic velocity, ΔV is the RVE-cell volume (large enough to guarantee sufficient smoothing, but not larger than a fraction of the mean gradient scale) while ΔV_f is the fluid part of the RVE cell, $\mathbf{u}$ is the RVE-averaged mean velocity (mean Darcy velocity, or volume flow velocity, essentially) and $\mathbf{u}^i$ is the RVE-averaged mean interstitial velocity. Note that for all these purposes, it is sufficient to define $\mathbf{u}^i$ as $\mathbf{u}^i = \mathbf{u}/\varepsilon_p$. For the velocity gradients we assume

$$\frac{\partial u_j}{\partial x_k} = \varepsilon_p \frac{\partial u^i_j}{\partial x_k} \tag{3-211}$$

where deviations from this expression (Ref. 30) are lumped into the modeled extra contributions. Turbulence kinetic energy and turbulence dissipation rate obey the same averaging and scaling rules as mean velocity

$$k = \varepsilon_p k^i, \quad \varepsilon = \varepsilon_p \varepsilon^i \tag{3-212}$$

At the same time, for the turbulence-specific dissipation rate and turbulence viscosity we take, by definition,

$$\omega \equiv \omega^{\mathrm{i}} = \frac{1}{\Delta V_{\mathrm{f}}} \int_{\Delta V_{\mathrm{f}}} \overline{\omega^{\mathrm{micro}}}\, \mathrm{dV}, \quad \mu_{\mathrm{T}} \equiv \mu_{\mathrm{T}}{}^{\mathrm{i}} = \frac{1}{\Delta V_{\mathrm{f}}} \int_{\Delta V_{\mathrm{f}}} \overline{\mu_{\mathrm{T}}{}^{\mathrm{micro}}}\, \mathrm{dV} \tag{3-213}$$

This happens because ω and μ_{T} do not have a reasonable volumetrically spread interpretation. Next, the turbulence friction velocity is by definition scaled as

$$u_\tau = \sqrt{\varepsilon_{\mathrm{p}}}\, u^{\mathrm{i}}{}_\tau \tag{3-214}$$

which is consistent with the common scalings $(u_\tau)^2 \sim k$ and $\rho(u_\tau)^2 \sim \mu U / y_{\mathrm{wall}}$.

The pressure entering the equations is the RVE-smoothed pressure,

$$p = p^{\mathrm{i}} \tag{3-215}$$

which preserves the gauge-invariance property.

THE SET OF EQUATIONS

The momentum equation is essentially a Brinkman equation for the mean REV-averaged velocity but the viscous stress now includes turbulence viscosity:

$$\begin{aligned} \frac{\rho}{\varepsilon_{\mathrm{p}}}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\frac{\mathbf{u}}{\varepsilon_{\mathrm{p}}}\right) = {} & -\nabla p - \left(\kappa^{-1}\mu + \rho\beta|\mathbf{u}| + \frac{Q_{\mathrm{m}}}{\varepsilon_{\mathrm{p}}^2}\right)\mathbf{u} + \mathbf{F} + \\ & \nabla\cdot\left[\frac{\mu+\mu_{\mathrm{T}}}{\varepsilon_{\mathrm{p}}}\left\{(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right\}\right] \end{aligned} \tag{3-216}$$

The formal modification of the k-equation involves changing the convective term according to $\rho\mathbf{u}\cdot\nabla k \rightarrow \rho\mathbf{u}\cdot\nabla(k/\varepsilon_{\mathrm{p}})$ and adding production by the porous matrix $P_{k,\mathrm{pm}}$ to the shear production $P_k \rightarrow P_k + P_{k,\mathrm{pm}}$:

$$\rho\frac{\partial k}{\partial t} + \rho\mathbf{u}\cdot\nabla\frac{k}{\varepsilon_{\mathrm{p}}} = \nabla\cdot\left(\left(\mu + \frac{\mu_{\mathrm{T}}}{\sigma_k}\right)\nabla k\right) + P_k + P_{k,\,\mathrm{pm}} - \rho\varepsilon \tag{3-217}$$

while the shear production is modified as

$$P_k = \frac{\mu_{\mathrm{T}}}{\varepsilon_{\mathrm{p}}}\left(\nabla\mathbf{u}:(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}(\nabla\cdot\mathbf{u})^2\right) - \frac{2}{3}\rho k\frac{\nabla\cdot\mathbf{u}}{\varepsilon_{\mathrm{p}}} \tag{3-218}$$

For the ε-equation, the changes are completely analogous: the convective term is modified according to $\rho\mathbf{u}\cdot\nabla\varepsilon \rightarrow \rho\mathbf{u}\cdot\nabla(\varepsilon/\varepsilon_{\mathrm{p}})$ and the turbulent dissipation rate production by the porous matrix $P_{\varepsilon,\mathrm{pm}}$ is added to the right-hand side:

$$\rho\frac{\partial\varepsilon}{\partial t}+\rho\mathbf{u}\cdot\nabla\frac{\varepsilon}{\varepsilon_p}=\nabla\cdot\left(\left(\mu+\frac{\mu_T}{\sigma_\varepsilon}\right)\nabla\varepsilon\right)+C_{\varepsilon1}\frac{\varepsilon}{k}P_k+P_{\varepsilon,\,pm}-C_{\varepsilon2}\rho\frac{\varepsilon^2}{k} \quad (3\text{-}219)$$

For ω-based models, the convective term changes as $\rho\mathbf{u}\cdot\nabla\omega\rightarrow(\rho\mathbf{u}/\varepsilon_p)\cdot\nabla\omega$ and the turbulent-specific dissipation rate production by the porous matrix $P_{\omega,pm}$ is added:

$$\rho\frac{\partial\omega}{\partial t}+\rho\frac{\mathbf{u}}{\varepsilon_p}\cdot\nabla\omega=\alpha\frac{\omega}{k}P_k+P_{\omega,\,pm}-\rho\beta\omega^2+\nabla\cdot((\mu+\sigma\mu_T)\nabla\omega) \quad (3\text{-}220)$$

The above modifications have been illustrated for the k-ε model and the ω-equation of the k-ω model, but are generally applicable to any two-equation turbulence model.

Calculation of turbulent viscosity via $\mu_T=l_{mix}\sqrt{k/\varepsilon_p}$ assumes that the following scaling should be applied:

$$l_{mix}=C_\mu\frac{k^{3/2}}{\varepsilon\sqrt{\varepsilon_p}} \quad (3\text{-}221)$$

or

$$l_{mix}=\frac{\sqrt{k/\varepsilon_p}}{\omega} \quad (3\text{-}222)$$

The realizable k-ε model needs the redefinition $C_\mu=\left(A_0+A_sU^{(*)}\frac{k}{\varepsilon\varepsilon_p}\right)^{-1}$.

For the Low Reynolds number k-ε model, $R_t=\rho k^2/(\mu\varepsilon\varepsilon_p)$ and $u_\varepsilon=(\mu\varepsilon/\rho/\varepsilon_p)^{1/4}$.

For the k-ω model, $\chi_k=\frac{1}{\omega^3\varepsilon_p}(\nabla k\cdot\nabla\omega)$, $\chi_\omega=\left|\Omega_{ij}\Omega_{jk}S_{ki}/(\beta_0^*\omega\varepsilon_p)^3\right|$. Analogously,

modifications to the θ_1, $CD_{k\omega}$, θ_2 coefficients of the SST model require substitution $k\rightarrow k/\varepsilon_p$.

The modifications to the ζ-equation of the v2-f model are the following: change convective term according to $\rho\mathbf{u}\cdot\nabla\zeta\rightarrow(\rho\mathbf{u}/\varepsilon_p)\cdot\nabla\zeta$, change $P_k\rightarrow P_k+P_{k,pm}$ in both terms on the right-hand side which contain P_k, and limit variable L by l_{pore}

$$L=\min\left(C_L\max\left[\frac{k^{3/2}}{\varepsilon},C_\eta\left(\frac{\nu^3}{\varepsilon}\right)^{1/4}\right],l_{pore}\right) \quad (3\text{-}223)$$

Wall Distance is now computed treating **Wall** and **Interior wall** adjacent to porous domains as usual solid walls.

In a RANS-RSM, $\mu_T\rightarrow\rho\,k/(\omega\,\varepsilon_p)$,Equation 3-216 is modified as

$$\nabla \cdot \left[\frac{\mu + \mu_T}{\varepsilon_p} \left\{ (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I} \right\} \right] \rightarrow \tag{3-224}$$
$$\nabla \cdot \left[\left(\frac{\mu}{\varepsilon_p} \left\{ (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I} \right\} - \rho \frac{\mathbf{R}}{\varepsilon_p} \right) \right]$$

The $\mathbf{R}$-equation follows the scaling of the k-equation Equation 3-217, taking into account transition to the tensor form, for example $P_{k,\mathrm{pm}} \rightarrow P_{R,\mathrm{pm}}$. The expressions Equation 3-68, Equation 3-69, Equation 3-190 and Equation 3-203 should be rewritten as

$$P_{ij} = -\rho\left(R_{ik}\frac{\partial U_j}{\partial x_k} + R_{jk}\frac{\partial U_i}{\partial x_k} \right) / \varepsilon_p \qquad P = -\rho R_{ij}\frac{\partial U_i}{\partial x_j} / \varepsilon_p \tag{3-225}$$

while in the pressure-strain expressions Equation 3-191 and Equation 3-204 strain-tensor and rotation-tensor should be substituted with

$$S_{ij} \rightarrow \frac{S_{ij}}{\varepsilon_p} \qquad \Omega_{ij} \rightarrow \frac{\Omega_{ij}}{\varepsilon_p} \tag{3-226}$$

ε-equation or ω-equation of a RANS-RSM follow the form of Equation 3-219 or Equation 3-220

with the corresponding changes to the evaluation of the model coefficients.

POROUS MEDIUM TURBULENCE MODEL

Porous medium turbulence model complements a basic turbulence model providing modeling for the above declared terms $P_{k,\mathrm{pm}}$ and $P_{\varepsilon,\mathrm{pm}}$, and $P_{\omega,\mathrm{pm}}$. The available modeling approaches are: **Default**, **Nakayama–Kuwahara**, and **Pedras–de Lemos**. **Default** and **Nakayama–Kuwahara** (Ref. 31) employ the following form of the porous production $P_{k,\mathrm{pm}}$ of turbulence kinetic energy

$$P_{k,\mathrm{pm}} = \rho\beta|\mathbf{u}|^3 \tag{3-227}$$

(where β is the non-Darcian coefficient from the Brinkman equation) while **Pedras–de Lemos** (Ref. 30) relies on

$$P_{k,\mathrm{pm}} = \frac{\rho C_{\mathrm{stpm}}|\mathbf{u}|}{\varepsilon_p l_{\mathrm{pore}}} k \tag{3-228}$$

For ε-based equations, **Default** and **Pedras–de Lemos** model the turbulence dissipation rate $P_{\varepsilon,\mathrm{pm}}$ as

$$P_{\varepsilon,\,\mathrm{pm}} = C_{\varepsilon 2,\,\mathrm{pm}} \frac{\rho C_{\mathrm{stpm}} |\mathbf{u}|}{\varepsilon_{\mathrm{p}} l_{\mathrm{pore}}} \varepsilon \tag{3-229}$$

while **Nakayama–Kuwahara** gives

$$P_{\varepsilon,\,\mathrm{pm}} = C_{\varepsilon 2,\,\mathrm{pm}} \frac{\rho \beta |\mathbf{u}|^4}{\varepsilon_{\mathrm{p}} l_{\mathrm{pore}}} \tag{3-230}$$

For the k-ω and SST models, **Default** and **Pedras–de Lemos** model porous production of the specific turbulent dissipation rate $P_{\omega,\mathrm{pm}}$ as

$$P_{\omega,\,\mathrm{pm}} = C_{\omega 2,\,\mathrm{pm}} \frac{\rho C_{\mathrm{stpm}} |\mathbf{u}|}{\varepsilon_{\mathrm{p}} l_{\mathrm{pore}}} \omega \tag{3-231}$$

while **Nakayama–Kuwahara** as

$$P_{\omega,\,\mathrm{pm}} = C_{\omega 2,\,\mathrm{pm}} \frac{\rho \beta |\mathbf{u}|^4}{\varepsilon_{\mathrm{p}} l_{\mathrm{pore}} k} \tag{3-232}$$

For ε-based models $C_{\varepsilon 2,\mathrm{pm}}$ is always the corresponding $C_{\varepsilon 2}$ coefficient entering ε-equation (that is, $C'_{\varepsilon 2}$ for v2-f). **Default** and **Pedras–de Lemos** have $C_{\omega 2,\mathrm{pm}} = \beta_0 / \beta_0^*$ for k-ω and $C_{\omega 2,\mathrm{pm}} = \beta / \beta_0^*$ for SST, while **Nakayama–Kuwahara** has $C_{\omega 2,\mathrm{pm}} = \beta_0 / \beta_0^{*2}$ for k-ω and $C_{\omega 2,\mathrm{pm}} = \beta / \beta_0^{*2}$ for SST.

Essentially, **Default** uses $P_{k,\mathrm{pm}}$ in the form proposed by Nakayama–Kuwahara and $P_{\varepsilon,\mathrm{pm}}$ or $P_{\omega,\mathrm{pm}}$ in the form proposed by Pedras–de Lemos. Since $\rho\beta|\mathbf{u}|^3$ actually is turbulence dissipation caused by the porous matrix, **Default** and **Nakayama–Kuwahara** are conservative models so that the k-equation guarantees that in a dense porous medium the specific turbulence dissipation achieves its limiting value

$$\varepsilon \to \beta |\mathbf{u}|^3 \tag{3-233}$$

The ε-equation, and ω-equation, of all the three models as well as the k-equation of Pedras-de Lemos ensure that the turbulence frequency in a dense porous matrix would approach its limiting value

$$\frac{\varepsilon}{k} \to \frac{C_{\mathrm{stpm}} |\mathbf{u}|}{\varepsilon_{\mathrm{p}} l_{\mathrm{pore}}} \tag{3-234}$$

Thus, **Default** and **Nakayama–Kuwahara** also ensure that in a dense porous matrix

$$k \to \frac{\varepsilon_p \beta |\mathbf{u}|^2 l_{\text{pore}}}{C_{\text{stpm}}} \tag{3-235}$$

However, **Pedras–de Lemos** then becomes a degenerate model with two identical equations, and the limiting values of k and ε might depend on the initial and boundary conditions in an uncontrollable way.

The coefficient C_{stpm}, which we call a **Coefficient of subgrid turbulence generation by porous matrix**, is equal to 0.212 by default as given in Ref. 31. However for **Pedras-de Lemos** it can be set to predefined **Original** value $0.28 \cdot \sqrt{\varepsilon_p}$ or **Recalibrated** value 0.18. Both are based using Equation 3-234 to match limiting values of ε/k, obtained using pore resolving simulations in dense porous matrix at different ε_p, with C_{stpm}. **Original** refers to Ref. 30 usage $C_{\text{stpm}} = c_k \sqrt{\varepsilon_p}$ while **Recalibrated** refers to the current convention when C_{stpm} is considered as independent of porosity.

For a RANS-RSM, $P_{k,\text{pm}}$ and $P_{\varepsilon,\text{pm}}$ and $P_{\omega,\text{pm}}$ are computed according to the above formulas, and then $P_{R,\text{pm}}$ is set to

$$P_{R,\,\text{pm}} = P_{k,\,\text{pm}} \frac{2}{3} \delta_{ij} \tag{3-236}$$

when **Production of Reynolds stresses by porous matrix** is **Isotropic** (default) and set to

$$P_{R,\,\text{pm}} = 2 P_{k,\,\text{pm}} \frac{u_i u_j}{|\mathbf{u}|^2} \tag{3-237}$$

when it is **Streamwise**.

Default and **Pedras–de Lemos** have $c_{\omega 2,\text{pm}} = \beta_{0W}/\beta_0^*$ for Wilcox R-ω and $c_{\omega 2,\text{pm}} = \beta_\omega / C_\mu$ for SSG-LRR, while **Nakayama–Kuwahara** has $c_{\omega 2,\text{pm}} = \beta_{0W}/\beta_0^{*2}$ for Wilcox R-ω and $c_{\omega 2,\text{pm}} = \beta_\omega / C_\mu^2$ for SSG-LRR.

WALL TREATMENT

Wall treatment essentially inherits wall treatment of a corresponding basic turbulence model. The main modification is due to the need to determine if at $\delta_w = h_w/2$ the turbulent log-layer still dominates (pores are resolved) or the limit of the dense porous matrix is reached (pores not resolved). The intermediate cases should be blended properly. In the current approach it is achieved by introducing an indicator function ind_{pmLL},which quantifies porous matrix dominance over the log-layer and is modeled as

$$\text{ind}_{\text{pmLL}} = 1 - e^{-\delta_w / l_{\text{pore}}} \tag{3-238}$$

Thus, at the wall (or rather the lift-off position) a variable ϕ (like traction, turbulence dissipation rate or turbulence specific dissipation rate) is determined as

$$\phi_w = (1 - \text{ind}_{\text{pmLL}})\phi_{\text{LL}} + \text{ind}_{\text{pmLL}}\phi_{\text{pm}} \tag{3-239}$$

where ϕ_{LL} and ϕ_{pm} are log-layer and dense porous matrix expressions, respectively.

Formally, the nonporous flow expression for traction should be multiplied by $(1 - \text{ind}_{\text{pmLL}})/\varepsilon_p$ because traction in the porous matrix is negligible due to homogenization of the gradients.

Wall Functions

The modifications are:

$$\delta_w^+ = \max\left(\frac{h}{2}\frac{\rho C_\mu^{1/4}\sqrt{k}}{\mu\sqrt{\varepsilon_p}}, 11.06\right),\ \delta_w = \frac{\delta_w^+ \mu\sqrt{\varepsilon_p}}{\rho u_\tau},\ u^+ = \sqrt{\varepsilon_p}\left(\frac{\ln(\delta_w^+)}{\kappa_v} + B\right) \tag{3-240}$$

where for the Realizable k-ε $C_\mu \to 1/(A_0 + 7.1)$ and for k-ω $C_\mu \to \beta_0^*$ (also in expressions below), while expression for the friction velocity u_τ is the same, and the traction is

$$\mathbf{n}\cdot\mathbf{K} - (\mathbf{n}\cdot\mathbf{K}\cdot\mathbf{n})\mathbf{n} = -(1 - \text{ind}_{\text{pmLL}})\frac{\rho u_\tau}{\varepsilon_p}\frac{\mathbf{u}}{u^+} \tag{3-241}$$

The wall value of ε is now

$$\varepsilon_w = (1 - \text{ind}_{\text{pmLL}})\frac{C_\mu^{3/4}k^{3/2}}{\kappa_v \delta_w \sqrt{\varepsilon_p}} + \text{ind}_{\text{pmLL}}\frac{C_{\text{stpm}}U_\parallel k}{\varepsilon_p l_{\text{pore}}} \tag{3-242}$$

representing blending of a log-layer value with a dense porous matrix value. The analogous expression for ω is:

$$\omega_w = (1 - \text{ind}_{\text{pmLL}})\frac{\rho k}{\kappa_v \delta_w^+ \mu \varepsilon_p} + \text{ind}_{\text{pmLL}}\frac{C_{\text{stpm}}U_\parallel}{\beta_0^* \varepsilon_p l_{\text{pore}}} \tag{3-243}$$

and also models transition from an asymptotic log-layer asymptotic to the dense porous matrix value.

The postprocessing variable for friction velocity $u_{\tau w}$ (`u_tauWall`) is based on the effective interstitial traction at the wall and is defined as

$$u_{\tau w} = \sqrt{(1 - \text{ind}_{\text{pmLL}})\frac{u_\tau}{\varepsilon_p}\frac{|\mathbf{u}|}{u^+}}$$

while the postprocessing variable for wall lift-off Δ_w^+ (`Delta_wPlus`) formally does not require modification of the definition

$$\Delta_w^+ = \max\left(\frac{\rho}{\mu}\frac{h_w}{2}u_{\tau w}, 11.06\right)$$

Automatic Wall Treatment

Now $u_\tau^{\log}$ and $\delta_w{}^+$ are modified as

$$u_\tau^{\log} = \frac{U_{\parallel}/\sqrt{\varepsilon_p}}{\frac{1}{\kappa_v}\log(\delta_w^+) + B}, \quad \delta_w^* = \frac{u^*\delta_w}{\nu\sqrt{\varepsilon_p}} \tag{3-244}$$

while the definitions of u_τ^{visc}, $u^{*,\log}$, u_τ, and u^* remain the same.

The traction is written as

$$\mathbf{n}\cdot\mathbf{K} - (\mathbf{n}\cdot\mathbf{K}\cdot\mathbf{n})\mathbf{n} = -(1 - \text{ind}_{\text{pmLL}})\frac{\rho u^*}{\varepsilon_p}\frac{\mathbf{u}}{u^+} \tag{3-245}$$

For the Low-Reynolds Number model further modifications are

$$\text{Re}_y = \frac{\delta_w\sqrt{k}}{\nu\sqrt{\varepsilon_p}} \tag{3-246}$$

$$\varepsilon_w = (1 - \text{ind}_{\text{pmLL}})\frac{k^{3/2}}{l_\varepsilon\sqrt{\varepsilon_p}} + \text{ind}_{\text{pmLL}}\frac{C_{\text{stpm}}U_{\parallel}k}{\varepsilon_p l_{\text{pore}}} \tag{3-247}$$

For v2-f model the further modifications are

$$\text{Re}_y = \frac{(C_{\mu v2f}\zeta_0)^{3/4}\sqrt{k}L}{2\nu\sqrt{\varepsilon_p}} \tag{3-248}$$

$$\varepsilon_w = (1 - \text{ind}_{\text{pmLL}})\frac{(C_{\mu v2f}\zeta_0)^{3/4}k^{3/2}}{l_\varepsilon\sqrt{\varepsilon_p}} + \text{ind}_{\text{pmLL}}\frac{C_{\text{stpm}}U_{\parallel}k}{\varepsilon_p l_{\text{pore}}} \tag{3-249}$$

For k-ω and SST models ω_{visc} does not change and the further modifications are

$$\omega_{\log} = \frac{u_\tau}{\sqrt{\beta_0^*}\kappa_v \delta_w \sqrt{\varepsilon_p}} \tag{3-250}$$

$$\omega = (1 - \mathrm{ind}_{\mathrm{pmLL}})\sqrt{\omega_{\mathrm{visc}}^2 + \omega_{\log}^2} + \mathrm{ind}_{\mathrm{pmLL}} \frac{C_{\mathrm{stpm}} U_{\parallel}}{\beta_0^* \varepsilon_p l_{\mathrm{pore}}} \tag{3-251}$$

The postprocessing variable for friction velocity $u_{\tau w}$ (`u_tauWall`) is based on the effective interstitial traction at the wall and is defined as

$$u_{\tau w} = \sqrt{(1 - \mathrm{ind}_{\mathrm{pmLL}}) u_\tau u^* / \varepsilon_p}$$

while the postprocessing variable for the resulting wall resolution, Δ_w^+ (`Delta_wPlus`), does not require a modification to its definition

$$\Delta_w^+ = \frac{u_{\tau w} \delta_w}{\nu}$$

Low-Re Wall Treatment

Low Reynolds number treatment is formally identical to the usual clear flow **Low Re** treatment. Strictly speaking, it is applicable only in case if the pore cell is fully resolved by the mesh. Otherwise the first computational cell is in the porous matrix but common clear flow $\mathbf{u} = 0$, $k = 0$ ($\mathbf{R} = 0$ for a RANS-RSM) conditions are applied. Thus, the behavior in several near-wall cells would be not correct.

BUOYANCY-INDUCED TURBULENCE

The two definitions of the production of turbulence kinetic energy by buoyancy, **User defined** and **Automatic from multiphysics**, become modified in porous domains as

$$P_{kb}^{\mathrm{Ud}} = -\varepsilon_p \frac{\mu_T g_i}{\sigma_T \bar{\rho}} \frac{\partial \bar{\rho}}{\partial x_i}, \quad P_{kb}^{\mathrm{Afm}} = \alpha_p \varepsilon_p \frac{\mu_T}{Pr_T} g_i \frac{\partial \tilde{T}}{\partial x_i} \tag{3-252}$$

Since $P_{kb} = P_{kb,\mathrm{mul}} k$, so

$$P_{kb,\,\mathrm{mul}}^{\mathrm{Ud}} = -\frac{l_{\mathrm{mix}}}{\sigma_T \sqrt{k/\varepsilon_p}} \frac{g_i}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial x_i}, \quad P_{kb,\,\mathrm{mul}}^{\mathrm{Afm}} = \alpha_p \frac{l_{\mathrm{mix}}}{Pr_T \sqrt{k/\varepsilon_p}} g_i \frac{\partial \tilde{T}}{\partial x_i} \tag{3-253}$$

A GENERAL REMARK ON SCALING WITH POROSITY

All the equations in porous medium presented above can be rewritten in terms of the mean interstitial quantities $\mathbf{u}^{\mathrm{i}}$, k^{i}, ε^{i}, ω^{i}. If we assume constant ε_p and multiply k-

equation and ε-equation by ε_p, then porosity ε_p would disappear from all the equations and they would look identical to the original clear flow equations. The additional terms (Darcy and Forchheimer in the momentum equation, and the above introduced extra productions in the turbulence equations) would contain the geometrical information about porous medium only via l_{pore}. This reasoning is naturally extended to all the boundary conditions. Also, all the numerous nondimensional intermediate variables which enter turbulence equations, for example R_t in the Low-Re k-ε model, should be scaled properly. Then, since scaling does not effect length and time, all the intermediate lengths, frequencies, and viscosities should be physical.

For example, the Burke–Plummer model follows this rule, while an approach introducing Forchheimer coefficient is consistent if the scaling

$$c_F = \frac{\tilde{c}_F}{\varepsilon_p^{3/2}} \tag{3-254}$$

is assumed with $\tilde{c}_F$ being considered as a constant.

Note that the friction velocity u_τ does not have an immediate interstitial meaning and, therefore, deviates from this scaling.

Inlet Values for the Turbulence Length Scale and Turbulent Intensity

If inlet data for the turbulence variables are not available, crude approximations for k, ε, ω, and ζ can be obtained from the following formulas:

$$\begin{aligned} k &= \frac{3}{2}(|\mathbf{U}|I_T)^2 \\ \varepsilon &= C_\mu^{3/4}\frac{k^{3/2}}{L_T} \\ \omega &= \frac{\sqrt{k}}{(\beta_0^*)^{1/4}L_T} \\ \zeta &= \frac{2}{3} \end{aligned} \tag{3-255}$$

where I_T is the turbulent intensity and L_T is the turbulence length scale. For a RANS-RSM, the default approximation of R_{ij} is

$$R_{ij} = (|\mathbf{U}|I_T)^2\delta_{ij} \tag{3-256}$$

A value of 10^{-3} (0.1%) is a low turbulent intensity I_T. Good wind tunnels can produce values as low as $5{\cdot}10^{-4}$ (0.05%). Fully turbulent flows usually have intensities between 0.05 (5%) and 0.1 (10%).

The turbulence length scale L_T is a measure of the size of the eddies that are not resolved. For free-stream flows these are typically very small (on the order of centimeters). The length scale cannot be zero, however, because that would imply infinite dissipation. Use Table 3-6 as a guideline when specifying L_T (Ref. 3) where l_w is the wall distance, and

$$l_w^+ = l_w / l^*$$

TABLE 3-6: TURBULENCE LENGTH SCALES FOR TWO-DIMENSIONAL FLOWS.

FLOW CASE	L_T	L
Mixing layer	$0.07L$	Layer width
Plane jet	$0.09L$	Jet half width
Wake	$0.08L$	Wake width
Axisymmetric jet	$0.075L$	Jet half width
Boundary layer ($\partial p/\partial x = 0$) – Viscous sublayer and log-layer – Outer layer	$\kappa l_w(1 - \exp(-l_w^+/26))$ $0.09L$	Boundary layer thickness
Pipes and channels (fully developed flows)	$0.07L$	Pipe diameter or hydraulic diameter or channel width

Theory for Buoyancy-Induced Turbulence

When the flow is compressible or weakly compressible, an additional contribution to the production of turbulent kinetic energy may be added. This contribution can be expressed in terms of Favre-averaged fluctuations or conventional time-filtered fluctuations according to,

$$P_{kb} = -\overline{u_i''}\frac{\partial \bar{p}}{\partial x_i} = \frac{\overline{\rho' u_i'}}{\bar{\rho}}\frac{\partial \bar{p}}{\partial x_i} \approx \overline{\rho' u_i'} g_i \qquad (3\text{-}257)$$

where g_i is the gravitational acceleration and the last approximation is applicable for small Froude numbers. Applying a gradient-diffusion modeling approach, Equation 3-257 can be recast into,

$$P_{kb} = -\frac{\mu_T}{\sigma_T}\frac{g_i}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial x_i} \tag{3-258}$$

where σ_T is the turbulent Schmidt number. The production term in the ε equation is derived from the production term in the k equation. Hence, the corresponding term in the ε equation becomes,

$$P_{\varepsilon b} = C_{\varepsilon 1}\frac{\varepsilon}{k}\max(P_{kb}, 0)\sin\theta \tag{3-259}$$

where $C_{\varepsilon 1}$ is the corresponding constant for every model (1.44 for the Realizable k-ε model). For the v2-f model ε/k is changed to τ^{-1}. θ is the angle between **u** and **g**, accounting for the difference between buoyant vertical shear layers and buoyant horizontal shear layers:

$$\sin\theta = \sqrt{1 - \left(\frac{\mathbf{u}\cdot\mathbf{g}}{|\mathbf{u}|\cdot|\mathbf{g}|}\right)^2}\cdot \operatorname{sgn}(\mathbf{u}\cdot\mathbf{g}) \tag{3-260}$$

Using the relation between k, ε, and ω, the buoyancy production term in the ω equation of the k-ω model can be derived as,

$$P_{\omega b} = \frac{\omega}{k}[(\alpha + 1)\max(P_{kb}, 0)\sin\theta - P_{kb}] \tag{3-261}$$

For the SST-model, the buoyancy production term is

$$P_{\omega b} = \frac{\rho}{\mu_T}[(\gamma_\omega + 1)\max(P_{kb}, 0)\sin\theta - P_{kb}] \tag{3-262}$$

Hence, the expressions for the various ε based and ω based turbulence models differ only in terms of constants and damping functions.

The v2-f turbulence model uses the gradient of the wall distance variable l_w to compute the wall-normal direction, and relating the wall-normal turbulent fluctuations to the direction of gravity results in the following expression for buoyant production of ζ,

$$P_{\zeta b} = \left(2\frac{|\mathbf{g}\cdot\nabla l_w|}{|\mathbf{g}|\cdot|\nabla l_w|} - \zeta\right)\frac{P_{kb}}{k} \tag{3-263}$$

This modeling assumes that the buoyancy-induced turbulence kinetic energy is pumped into the component of k aligned with **g**.

When the buoyancy contribution is determined from a multiphysics node, density variations with respect to the variable in the coupled physics interface are considered. Currently, this option is available for nonisothermal flow when the coupled interface is a Heat Transfer in Fluids interface, and, Equation 3-258 is then replaced by

$$P_{kb} = \alpha_p \frac{\mu_T}{Pr_T} g_i \frac{\partial \tilde{T}}{\partial x_i} \tag{3-264}$$

When coupling to other physics, a user-defined Schmidt number should be applied.

Theory for the Pressure, No Viscous Stress Boundary Condition

For this module, the turbulent intensity I_T, turbulence length scale L_T, and reference velocity scale U_{ref} values are related to the turbulence variables via

$$k = \frac{3}{2}(I_T U_{ref})^2, \quad \varepsilon = \frac{C_\mu^{3/4}}{L_T}\left(\frac{3(I_T U_{ref})^2}{2}\right)^{\frac{3}{2}}, \quad \omega = \sqrt{\frac{3}{2}}\frac{I_T U_{ref}}{(\beta_0^*)^{1/4} L_T}, \quad \zeta = \frac{2}{3}$$

For recommendations of physically sound values see Inlet Values for the Turbulence Length Scale and Turbulent Intensity.

Also see Inlet and Outlet for the node settings.

Initial Values for Generate New Turbulence Model Interfaces

A major advantage with the **Generate New Turbulence Model Interface** feature is that it can express initial values for the new turbulence model in terms of the original model. This makes it possible to first solve a problem using a simple, but robust, turbulence model, such as the k-ε model, and then switch to a more advanced model.

Unless the **Initial value from study** is **None**, the **Generate New Turbulence Model Interface** initial values for velocity and pressure are taken directly from the solution of the parent model. The initial values of turbulent dependent variables are estimated using the solution from the selected study:

- When the parent model is a Laminar Flow model, or when **Initial value from study** is **None**, turbulent dependent variables get their default initial values.

- Initial values of dependent variables that exist in both the parent model and the generated model are taken directly from the selected study.
- When the parent model is Turbulent Flow, Wilcox R-ω or Turbulent Flow, SSG-LRR and the generated model has Dependent Variable k, its initial value is

$$k_{\text{init}} = (uu + vv + ww)/2$$

  It is also implied that this value of k is used when a RANS-EVM is generated from a RANS-RSM
- When Wilcox R-ω or SSG-LRR is generated from a RANS-EVM

$$R_{ij} = \frac{2}{3}k\delta_{ij} - \frac{\nu_T}{\mu_T + \mu}K_{ij}$$

  where K_{ij} is the K_stress_tensor variable, while k is the Dependent Variable of the parent model if it exists or k_{init} otherwise
- When the parent model is Turbulent Flow, k-ε or Turbulent Flow, Low Reynolds k-ε or v2-f and the generated model is Turbulent Flow, k-ω or SST or Wilcox R-ω or SSG-LRR, the initial value of ω is

$$\omega_{\text{init}} = \rho k/\mu_T$$

- When the parent model is k-ω or SST or Wilcox R-ω or SSG-LRR, and the generated model is k-ε or Low Reynolds k-ε or v2-f (for v2-f C_μ is replaced by $(2/3)C_{\mu\text{-v2f}}$), the initial value of ε is

$$\varepsilon_{\text{init}} = C_\mu \rho k^2/\mu_T$$

- When the parent model is Algebraic yPlus, and the generated model is k-ε, Low Reynolds k-ε or v2-f (for v2-f C_μ is replaced by $(2/3)C_{\mu\text{-v2f}}$), the initial values of k and ε are:

$$k_{\text{init}} = \nu_T^2/(\sqrt{C_\mu}L_T^2)$$

$$\varepsilon_{\text{init}} = (C_\mu^{3/4}/L_T)k_{\text{init}}^{3/2}$$

  where $L_T = \max(\kappa_a y, (y^*\upsilon)/u_\tau)$ and $u_\tau = |\mathbf{u}|/u^+$.
- When the parent model is Algebraic yPlus and the generated model is k-ω or SST or Wilcox R-ω or SSG-LRR, the initial values of k and ω are

$$k_{\text{init}} = \nu_T^2/(\sqrt{\beta_0^*}L_T^2)$$

$$\omega_{\text{init}} = \sqrt{k_{\text{init}}}/(\beta_0^{*1/4}L_T)$$

- When the parent model is L-VEL, and the generated model is k-ε, Low Reynolds k-ε or v2-f (for v2-f C_μ is replaced by $(2/3)C_{\mu\,-\text{v2f}}$), the initial values of k and ε are

$$k_{\text{init}} = \nu_T^2/(\sqrt{C_\mu}L_T^2)$$

$$\varepsilon_{\text{init}} = (C_\mu^{3/4}/L_T)k_{\text{init}}^{3/2}$$

  where $L_T = \max(\kappa_l y, (\kappa_l \upsilon E_l)/u_\tau)$.
- When the parent model is L-VEL, and the generated model is k-ω and SST or Wilcox R-ω or SSG-LRR, the initial values of k and omega are

$$k_{\text{init}} = \nu_T^2/(\sqrt{\beta_0^*}L_T^2)$$

$$\omega_{\text{init}} = \sqrt{k_{\text{init}}}/(\beta_0^{*1/4}L_T)$$

- When the parent model is Spalart–Allmaras and the generated model is k-ε, Low Reynolds k-ε or v2-f (for v2-f C_μ is replaced by $(2/3)C_{\mu\,-\text{v2f}}$), the initial value of k and ε are:

$$k_{\text{init}} = \frac{f_{v1}^2}{\sqrt{C_\mu}} \cdot \min\left(\left(\frac{\tilde{\nu}}{\kappa_\nu y}\right)^2, \nu|\Omega|\right)$$

$$\varepsilon_{\text{init}} = \frac{\chi^8}{(\chi^3 + c_{v1}^3)^3} \cdot \min\left(\frac{1}{\nu}\left(\frac{\tilde{\nu}}{\kappa_\nu y}\right)^4, \nu|\Omega|^2\right)$$

- When the parent model is Spalart–Allmaras and the generated model is k-ω, SST, Wilcox R-ω, or SSG-LRR the initial values of k and ω are

$$k_{\text{init}} = \frac{f_{v1}^2}{\sqrt{\beta_0^*}} \cdot \min\left(\left(\frac{\tilde{\nu}}{\kappa_v y}\right)^2, \nu|\Omega|\right)$$

$$\omega_{\text{init}} = \frac{1}{\sqrt{\beta_0^*}} \frac{\chi^2}{\chi^3 + c_{v1}^3} \cdot \min\left(\frac{1}{\nu}\left(\frac{\tilde{\nu}}{\kappa_v y}\right)^2, |\Omega|\right)$$

- When the generated model is Spalart–Allmaras turbulent mode, and the parent model any turbulence model but Spalart–Allmaras, the initial value of the dependent variable is $\nu_{\text{init}} = \mu_T/\rho$.

Solvers for Turbulent Flow

The nonlinear system that the Navier–Stokes (RANS) and turbulence transport equations constitute can become ill-conditioned if solved using a fully coupled solver. Turbulent flows are therefore solved using a segregated approach (Ref. 21): Navier–Stokes in one group and the turbulence transport equations in another.

For each iteration in the Navier–Stokes group in stationary simulations, three iterations are performed for the turbulence transport equations. This is necessary to make sure that the very nonlinear source terms in the turbulence transport equations are in balance before performing another iteration for the Navier–Stokes group.

The default iterative solver for the turbulence transport equations is a damped Newton method with constant damping factor. In each iteration, a linearized version of the nonlinear system is solved using GMRES accelerated by Smoothed Aggregated Algebraic Multigrid (SAAMG). The default smoother is SOR Line.

As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, Geometric Multigrid (GMG) requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared memory computations with many cores.

- Pseudo Time Stepping for Turbulent Flow Models
- Multigrid, Stationary Solver, Iterative, and SOR Line in the *COMSOL Multiphysics Reference Manual*

Pseudo Time Stepping for Turbulent Flow Models

The default stationary solver applies pseudo time stepping for both 2D and 3D models. This improves the robustness of the nonlinear iterations as well as the condition number for the linear equation system. The latter is especially important for large 3D models where iterative solvers must be applied. The turbulence equations use the same $\Delta\tilde{t}$ as the momentum equations.

The default manual expression for $\mathrm{CFL}_{\mathrm{loc}}$ is, for 2D models:

$$1.3^{\min(\mathrm{niterCMP}-1,\,9)} + \mathrm{if}(\mathrm{niterCMP} > 25,\, 9 \cdot 1.3^{\min(\mathrm{niterCMP}-25,\,9)},\, 0) + \mathrm{if}(\mathrm{niterCMP} > 50,\, 90 \cdot 1.3^{\min(\mathrm{niterCMP}-50,\,9)},\, 0)$$

and for 3D models:

$$1.3^{\min(\mathrm{niterCMP}-1,\,9)} + \mathrm{if}(\mathrm{niterCMP} > 30,\, 9 \cdot 1.3^{\min(\mathrm{niterCMP}-30,\,9)},\, 0) + \mathrm{if}(\mathrm{niterCMP} > 60,\, 90 \cdot 1.3^{\min(\mathrm{niterCMP}-60,\,9)},\, 0)$$

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Theory for the Large Eddy Simulation Interfaces

Large Eddy Simulations offer an alternative approach to turbulent flow simulations as compared to the RANS approach (see Theory for the Turbulent Flow Interfaces). In LES, the larger three-dimensional, unsteady eddies are resolved, whereas the effect of the smaller eddies is modeled. This requires the simulations to be three-dimensional and time dependent. The velocity, pressure and temperature fields are divided into resolved, ($\mathbf{u}$, p, T), and unresolved, ($\mathbf{u}'$, p', T'), scales. The unresolved scales are assumed to be orthogonal to the inner-product space of the resolved scales and to vanish on $\partial\Omega$, the boundaries of the domain Ω, (see Ref. 1 for further details).

Inserting the variable decomposition into the conservative forms of the continuity, momentum and energy equations yields

$$\begin{gathered}
\frac{\partial(\rho+\rho')}{\partial t}+\nabla\cdot[(\rho+\rho')(\mathbf{u}+\mathbf{u}')]=0\\
\frac{\partial[(\rho+\rho')(\mathbf{u}+\mathbf{u}')]}{\partial t}+\nabla\cdot[(\rho+\rho')(\mathbf{u}+\mathbf{u}')\otimes(\mathbf{u}+\mathbf{u}')]=\\
\nabla\cdot[-(p+p')\mathbf{I}+\mathbf{K}+\mathbf{K}']\\
\frac{\partial}{\partial t}\left[(\rho+\rho')\left(e+e'+\frac{1}{2}\|\mathbf{u}+\mathbf{u}'\|^2\right)\right]+\nabla\cdot\left[(\rho+\rho')(\mathbf{u}+\mathbf{u}')\left(h+h'+\frac{1}{2}\|\mathbf{u}+\mathbf{u}'\|^2\right)\right]=\\
\nabla\cdot[(\mathbf{u}+\mathbf{u}')\cdot(\mathbf{K}+\mathbf{K}')-(\mathbf{q}+\mathbf{q}')]
\end{gathered}\tag{3-265}$$

Projecting Equation 3-265 onto the finite element subspaces for the resolved pressure, velocity and temperature scales, and neglecting the influence of unresolved scales on the diffusion coefficients for momentum and heat gives

$$
\begin{aligned}
&\left(\hat{p}, \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u})\right)_{\Omega} = (\nabla \hat{p}, \rho \mathbf{u}' + \rho'(\mathbf{u} + \mathbf{u}'))_{\Omega} \\
&\left(\hat{\mathbf{u}}, \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \cdot [(\rho + \rho')(\mathbf{u} + \mathbf{u}') \otimes (\mathbf{u} + \mathbf{u}') - \rho \mathbf{u} \otimes \mathbf{u}]\right)_{\Omega} = \\
&(\hat{\mathbf{u}}, -p\hat{\mathbf{n}} + \mathbf{K}\hat{\mathbf{n}})_{\partial\Omega} + (\nabla \hat{\mathbf{u}}, (p + p')\mathbf{I} - \mathbf{K})_{\Omega} \\
&\left(\hat{T}, \frac{\partial}{\partial t}\left[\rho\left(e + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] + \nabla \cdot \left[\rho \mathbf{u}\left(h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right]\right)_{\Omega} + \\
&\left(\hat{T}, \nabla \cdot \left[(\rho + \rho')(\mathbf{u} + \mathbf{u}')\left(h + h' + \frac{1}{2}\|\mathbf{u} + \mathbf{u}'\|^2\right) - \rho \mathbf{u}\left(h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right]\right)_{\Omega} = \\
&(\hat{T}, [\mathbf{u} \cdot \mathbf{K} - \mathbf{q}] \cdot \hat{\mathbf{n}})_{\partial\Omega} - (\nabla \hat{T}, (\mathbf{u} + \mathbf{u}') \cdot (\mathbf{K} + \mathbf{K}') - \mathbf{q})_{\Omega}
\end{aligned}
\tag{3-266}
$$

with the following thermodynamic relations

$$
\begin{aligned}
\rho &= f(p, T) \\
dh &= C_p dT + \frac{(1 - \alpha_p T)}{\rho} dp \\
e &= h - \frac{p}{\rho} \\
\alpha_p &= -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \\
\beta_T &= \frac{1}{\rho}\left(\frac{\partial \rho}{\partial p}\right)_T
\end{aligned}
\tag{3-267}
$$

From the second relation

$$
h = h(T_{\text{ref}}, p_{\text{ref}}) + \int_{T_{\text{ref}}}^{T} C_p dT + \int_{p_{\text{ref}}}^{p} \frac{(1 - \alpha_p T)}{\rho} dp = h_{\text{ref}} + \Delta h \tag{3-268}
$$

which together with the third relation can be used to further simplify the weak-form energy equation

$$
\begin{aligned}
&\left(\hat{T}, \frac{\partial}{\partial t}\left[\rho\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] + \nabla \cdot \left[\rho \mathbf{u}\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] - \frac{\partial p}{\partial t}\right)_{\Omega} + \\
&\left(\hat{T}, \nabla \cdot \left[(\rho + \rho')(\mathbf{u} + \mathbf{u}')\left(\Delta h + h' + \frac{1}{2}\|\mathbf{u} + \mathbf{u}'\|^2\right) - \rho \mathbf{u}\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right]\right)_{\Omega} = \\
&(\hat{T}, [\mathbf{u} \cdot \mathbf{K} - \mathbf{q}] \cdot \hat{\mathbf{n}})_{\partial\Omega} - (\nabla \hat{T}, (\mathbf{u} + \mathbf{u}') \cdot (\mathbf{K} + \mathbf{K}') - \mathbf{q})_{\Omega} \\
&-\left(\hat{T}, h_{\text{ref}}\left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u})\right]\right)_{\Omega} + (\nabla \hat{T}, h_{\text{ref}}[\rho \mathbf{u}' + \rho'(\mathbf{u} + \mathbf{u}')])_{\Omega}
\end{aligned}
\tag{3-269}
$$

If the pressure and temperature belong to the same inner-product space, the last line of Equation 3-269 becomes a constant multiple of the weak-form continuity equation, which is solved to numerical precision. In the current implementation, the subscale viscous work, $\mathbf{u} \cdot \mathbf{K}' + \mathbf{u}' \cdot (\mathbf{K} + \mathbf{K}')$, is neglected since $\mathbf{K}'$ cannot be resolved. This results in the following weak-form energy equation:

$$\begin{gathered}\left(\hat{T}, \frac{\partial}{\partial t}\left[\rho\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] + \nabla \cdot \left[\rho\mathbf{u}\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] - \frac{\partial p}{\partial t}\right)_\Omega + \\ \left(\hat{T}, \nabla \cdot \left[(\rho + \rho')(\mathbf{u} + \mathbf{u}')\left(\Delta h + h' + \frac{1}{2}\|\mathbf{u} + \mathbf{u}'\|^2\right) - \rho\mathbf{u}\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right]\right)_\Omega = \\ (\hat{T}, [\mathbf{u} \cdot \mathbf{K} - \mathbf{q}] \cdot \hat{\mathbf{n}})_{\partial\Omega} - (\nabla\hat{T}, \mathbf{u} \cdot \mathbf{K} - \mathbf{q})_\Omega\end{gathered} \tag{3-270}$$

The unresolved scales of density and enthalpy are modeled as

$$\begin{aligned}\rho' &= \rho\beta_T p' - \rho\alpha_p T' \\ h' &= C_p T' + \frac{(1 - \alpha_p T)}{\rho} p'\end{aligned} \tag{3-271}$$

The unresolved scales of the dependent variables are in turn modeled in terms of the equation residuals

$$\begin{aligned}p' &= -\tau_c \mathrm{res}_c \\ \mathbf{u}' &= -\tau_m \mathbf{res}_m \\ T' &= -\tau_e \mathrm{res}_e\end{aligned} \tag{3-272}$$

where the residuals are given by

$$\begin{aligned}\mathrm{res}_c &= \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) \\ \mathbf{res}_m &= \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla\mathbf{u}\right) + \nabla \cdot (p\mathbf{I} - \mathbf{K}) \\ \mathrm{res}_e &= \rho\left[\frac{\partial}{\partial t}\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right) + \mathbf{u} \cdot \nabla\left(\Delta h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] - \frac{\partial p}{\partial t} - \nabla \cdot (\mathbf{u} \cdot \mathbf{K} - \mathbf{q})\end{aligned} \tag{3-273}$$

and the intrinsic time scales are given by

$$\tau_c = C_1(\rho\tau_m \mathrm{trace}(\mathbf{G}))^{-1}$$
$$\tau_m = \frac{1}{\sqrt{\left(\frac{C_2\rho}{\Delta t}\right)^2 + 4\rho^2\mathbf{u}\cdot\mathbf{G}\mathbf{u} + C_3\mu^2\mathbf{G}:\mathbf{G}}} \tag{3-274}$$
$$\tau_e = \frac{1}{\sqrt{\left(\frac{C_2\rho C_p}{\Delta t}\right)^2 + 4\rho^2 C_p^2\mathbf{u}\cdot\mathbf{G}\mathbf{u} + C_4(\mathbf{k}\mathbf{G}):(\mathbf{k}\mathbf{G})}}$$

Here, C_1, C_3, and C_4 are constants depending on the order of the shape functions and the shape of the element, and C_2 is a constant depending on the temporal scheme. $\mathbf{G}$ is the covariant metric tensor, and $\mathbf{k}$ is the thermal-diffusion tensor.

When the **Use dynamic subgrid time scale** option is selected, the first terms under the square-roots in Equation 3-274 are replaced by estimates of inverse time scales based on time-derivatives of momentum and enthalpy. The **Limit small time steps effect on stabilization time scale** option is used to ramp out the time-derivative terms in Equation 3-273 and terms proportional to Δt^{-2} in Equation 3-274 when the time step becomes much smaller than what is required in LES (see Temporal resolution).

In certain cases, the residual-based Reynolds-stress contribution has been found to be too small (see Ref. 2). For this reason, the residual-based variational multiscale with viscosity (RBVMWV) method adds residual-based viscosity terms to the right-hand side of the weak-form momentum and energy equations in Equation 3-266,

$$-(\nabla\hat{\mathbf{u}},\ \rho\tilde{C}|\mathbf{u}'|h(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))_\Omega,\quad -\left(\nabla\hat{T},\ \frac{\rho C_p\tilde{C}|\mathbf{u}'|h}{\mathrm{Pr}_T}\nabla T\right)_\Omega \tag{3-275}$$

where $\tilde{C}$ is a model constant, and h is a measure of the element size.

For the Smagorinsky model, the terms $\nabla\cdot(\rho\mathbf{u}'\otimes\mathbf{u}'+\rho'\mathbf{u}'\otimes(\mathbf{u}+\mathbf{u}'))$ and $\nabla\cdot(\rho\mathbf{u}'h'+\rho'(\mathbf{u}+\mathbf{u}')h')$ in the weak-form momentum and energy equations are replaced by

$$\left(\nabla\hat{\mathbf{u}},\ 2\mu_T\left[\mathbf{S}-\frac{1}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right]\right)_\Omega,\quad \left(\nabla\hat{T},\frac{C_p\mu_T}{\mathrm{Pr}_T}\nabla T\right)_\Omega \tag{3-276}$$

where

$$\mu_T = \rho C_s^2|\mathbf{S}-\bar{\mathbf{S}}|/\mathrm{trace}(\mathbf{G}) \tag{3-277}$$

and

$$\mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \tag{3-278}$$

and $\bar{\mathbf{S}}$ is the projection of $\mathbf{S}$ onto the space of constant shape functions. This corresponds to a further decomposition of the resolved scales into large resolved scales and small resolved scales (see Ref. 3).

Note that all three models require equal-order interpolation for pressure, velocity and temperature.

WALL BOUNDARY CONDITION

Low Reynolds Number Wall Treatment

When **Wall treatment** is set to **Low Re**, a Dirichlet condition is imposed on the velocity field at the walls. Adequate resolution of the wall layers requires that $h_w \sim \nu/u_\tau$, where h_w is the thickness of the mesh cells next to the wall and $u_\tau = \sqrt{\tau_w/\rho}$ is the friction velocity based on the tangential stress τ_w at the wall.

Automatic Wall Treatment

When **Wall treatment** is set to **Automatic**, a Dirichlet condition is imposed on the wall-normal velocity component and a traction force is applied in the tangential direction opposite to the local velocity vector. To evaluate the magnitude, ρu_τ^2, of the traction force, the Reynolds number based on the magnitude of the tangential velocity and the normal distance, y, to the wall,

$$\mathrm{Re} = \frac{u_{\mathrm{tang}} y}{\nu} = \frac{u_{\mathrm{tang}}}{u_\tau} \cdot \frac{u_\tau y}{\nu} = u^+ y^+$$

is evaluated halfway between the wall and the first vertexes inside the domain, at $y = \delta_w$. Asymptotic solutions to the L-VEL equation (Equation 3-86) can be found for low and high values of the Reynolds number. For low values of the Reynolds number (inside the viscous wall layer),

$$u^+_{\mathrm{lin}} = \sqrt{\mathrm{Re}}$$

and for large values of the Reynolds number (inside the logarithmic layer),

$$u^+_{\mathrm{log}} = \frac{1}{\kappa}\left(1 - \frac{\log(\log(\kappa E \mathrm{Re}))}{1 + \log(\kappa E \mathrm{Re})}\right)\log(\kappa E \mathrm{Re})$$

The two expressions are blended according to

$$u^+ = ((u^+_{\text{lin}})^{-7} + (u^+_{\text{log}})^{-7})^{-1/7}$$

and the friction velocity is finally obtained from

$$u_\tau = \frac{u_{\text{tang}}}{u^+}$$

The **Automatic** option should be used with caution since boundary layers, especially on smooth surfaces, in many cases need to be resolved down to the top of the viscous wall layer ($y^+ \sim 5$). When the point of boundary-layer separation is known, such as for the flow around bodies with sharp edges, the **Automatic** option may be used to reduce the number of DOFs in the model. Automatic wall treatment for the energy equation is described in

When automatic wall treatment is applied in an LES model, a flux condition is imposed for the energy equation. The heat flux between the fluid with temperature T_f and a wall with temperature T_w, is

$$q_{\text{wf}} = \frac{\rho C_p u_\tau (T_w - T_f)}{T^+}$$

where T^+ is the dimensionless temperature, given by

$$T^+ = \text{Pr}\delta^+_w$$

for $\delta^+_w < \delta^*_w$ and

$$T^+ = \text{Pr}\delta^*_w + \frac{\text{Pr}_T}{\kappa}\log(\sqrt{1 + 4\kappa^2(\delta^+_w - \delta^*_w)^2} + 2\kappa(\delta^+_w - \delta^*_w))$$

$$- \begin{cases} \dfrac{(2\text{Pr}_T - \text{Pr})}{\kappa\sqrt{\dfrac{\text{Pr}}{\text{Pr}_T} - 1}} \tan^{-1}\left(\sqrt{\dfrac{\text{Pr}}{\text{Pr}_T} - 1}\,\dfrac{(\sqrt{1 + 4\kappa^2(\delta^+_w - \delta^*_w)^2} - 1)}{2\kappa(\delta^+_w - \delta^*_w)}\right), & \text{Pr} \geq \text{Pr}_T \\ \dfrac{(2\text{Pr}_T - \text{Pr})}{2\kappa\sqrt{1 - \dfrac{\text{Pr}}{\text{Pr}_T}}} \log\left(\dfrac{1 + \sqrt{1 - \dfrac{\text{Pr}}{\text{Pr}_T}}\,\dfrac{(\sqrt{1 + 4\kappa^2(\delta^+_w - \delta^*_w)^2} - 1)}{2\kappa(\delta^+_w - \delta^*_w)}}{1 - \sqrt{1 - \dfrac{\text{Pr}}{\text{Pr}_T}}\,\dfrac{(\sqrt{1 + 4\kappa^2(\delta^+_w - \delta^*_w)^2} - 1)}{2\kappa(\delta^+_w - \delta^*_w)}}\right), & \text{Pr} < \text{Pr}_T \end{cases}$$

for $\delta_w^+ \geq \delta_w^*$, where

$$\delta_w^* = \frac{1}{\kappa}\left(1 + \log\left(\frac{E}{4\kappa}\right)\right)$$

TEMPORAL RESOLUTION

Adequate resolution of the convective time scale requires that

$$\Delta t < 0.5 h_U / U$$

where h_U is the mesh size in the streamline direction. Larger values of Δt may lead to damping of turbulence and in some cases even convergence issues. The built-in variable `spf.dt_CFL` may be used to limit the maximum time step.

Synthetic Turbulence Inlet Condition

The methodology used for generating turbulent, fluctuating velocity field at the inlet boundary using Fourier series is described. A time correlation between such fields generated at successive time instances is provided.

INSTANTANEOUS VELOCITY FIELD

An instantaneous, turbulent, fluctuating velocity field, $\mathbf{U}'_{in}$, is generated at each time step of the simulation using random Fourier modes as

$$\mathbf{U}'_{in} = 2 \sum_{n=0}^{N-1} \hat{u}^n \cos(\beta^n) \sigma^n .$$

Here, N is the number of Fourier modes in the wave number space $\kappa_{max} - \kappa_{min}$. This space is divided into intervals of size $\Delta\kappa = (\kappa_{max} - \kappa_{min})/(N-1)$. The largest wavenumber, κ_{max}, is taken to be $2\pi/\Delta$, where Δ is the smallest element size in the inlet boundary, disregarding the boundary layer elements. The smallest wavenumber, κ_{min}, is taken to be κ_e/p. Here, $p = 5$ is chosen as a suitable value and $\kappa_e = (9\pi\alpha)/(55L_T)$, where $\alpha = 1.453$, the turbulent length scale $L_T = (C_\mu^{3/4} k_0^{3/2})/\varepsilon_0$, and $C_\mu = 0.09$ is the default value.

The quantity $\hat{u}^n$ is the amplitude of the nth mode. It is obtained from a modified von Kármán spectrum as,

$$\hat{u}^n = \sqrt{E(\kappa^n)\Delta\kappa},$$

$$E(\kappa^n) = 1.453\frac{u_{\text{rms}}^2}{\kappa_e}\frac{(\kappa^n/\kappa_e)^4}{[1+(\kappa^n/\kappa_e)^2]^{17/6}}\exp(-2(\kappa^n/\kappa_\eta))^2.$$

The quantity $\kappa_\eta = \varepsilon_0{}^{1/4}\nu^{-3/4}$, where, ν is the fluid kinematic viscosity. The root mean square velocity is calculated as $u_{\text{rms}} = \sqrt{2k_0/3}$. The components of the wavenumber vector for the nth mode are computed from random angles θ^n and ϕ^n as,

$$\kappa_1^n = (\kappa_{\min} + n\Delta\kappa)\sin(\theta^n)\cos(\phi^n),$$

$$\kappa_2^n = (\kappa_{\min} + n\Delta\kappa)\sin(\theta^n)\sin(\phi^n),$$

$$\kappa_3^n = (\kappa_{\min} + n\Delta\kappa)\cos(\theta^n).$$

The random angles are generated at each time step and for every Fourier mode such that the wave number vectors are uniformly distributed in the hemispherical shell, that is, $0 \le \theta^n \le 2\pi$ and $0 \le \phi^n \le \pi$. Additionally, the user may specify a seed value to be used in the generation of the random angles.

The phase angle $\beta^n = \kappa^n \cdot \mathbf{x} + \psi^n$, where the phase angle at the origin, ψ^n, is randomly generated, such that, $0 \le \psi^n \le 2\pi$.

The direction of the fluctuating velocity, σ^n, is chosen to be orthogonal to the wavenumber vector. Its orientation in the plane orthogonal to the wavenumber vector is determined by a random angle α^n, where $0 \le \alpha^n \le 2\pi$. It is given as,

$$\sigma_1^n = \cos(\phi^n)\cos(\theta^n)\cos(\alpha^n) - \sin(\phi^n)\sin(\alpha^n),$$

$$\sigma_2^n = \sin(\phi^n)\cos(\theta^n)\cos(\alpha^n) + \cos(\phi^n)\sin(\alpha^n),$$

$$\sigma_3^n = -\sin(\theta^n)\cos(\alpha^n).$$

TIME CORRELATIONS

At each time step, an instantaneous velocity field is generated as described in the previous section. Such velocity fields generated at successive time instances are totally independent of each other. To overcome this unphysical nature of the fluctuations, the following correlation in time is introduced. It provides a convenient way to prescribe the turbulent time scale of the fluctuations.

The fluctuating component of the prescribed inlet velocity at current time, $\mathbf{u}'_{\text{in,t}}$, is related to its value at the previous time, $\mathbf{u}'_{\text{in,(t}-\Delta\text{t)}}$, and the instantaneous velocity fluctuation, $\mathbf{U}'_{\text{in}}$, as

$$\mathbf{u}'_{\text{in,t}} = c_1\mathbf{u}'_{\text{in,(t-}\Delta\text{t)}} + c_2\mathbf{U}'_{\text{in}}.$$

The coefficients $c_1 = \exp(-\Delta t/T_{\text{int}})$ and $c_2 = \sqrt{1-c_1^2}$. Here, Δt is the time step size. The integral time scale is computed as $T_{\text{int}} = L_{\text{int}}/U_b$, where the integral length scale, L_{int}, is given by ${k_0}^{3/2}/\varepsilon_0$ and the bulk velocity, U_b, is the norm of the velocity averaged over the inlet boundary.

References for LES

1. Y. Bazilevs, V.M. Calo, J.A. Cottrell, T.J.R. Hughes, A. Reali, and G. Scovazzi, "Variational multiscale residual-based turbulence modeling for large eddy simulation of incompressible flows," *Comput. Methods Appl. Mech. Eng.*, vol. 197, pp. 173–201, 2007.

2. J. Liu, "Residual-based variational multiscale models for large eddy simulations of compressible and incompressible flows," *Rensselaer Polytechnic Institute*, PhD thesis, 2012.

3. J. Volker and K. Songul, "A finite element variational multiscale method for the Navier–Stokes equations," *SIAM J. Sci. Comput.*, vol. 26, no. 5, pp. 1485–1503, 2005.

4. L. Davidson, "Using isotropic synthetic fluctuations as inlet boundary conditions for unsteady simulations," *Adv. Appl. Fluid Mech.*, vol. 1, no. 1, pp. 1–35, 2007.

Theory for the Detached Eddy Simulation Interfaces

Detached Eddy Simulation combines Large Eddy Simulation and RANS, resolving the large turbulent eddies in the bulk and modeling the unresolved eddies, in the bulk using a LES approach, and in the near-wall region using a RANS approach. As for LES, the simulations must be three-dimensional and time dependent. Turbulent stresses, modeled by a Boussinesq closure, are added to the existing LES models using the Spalart–Allmaras model (see The Turbulent Flow, Spalart–Allmaras Interface), and the wall distance in the transport equation for $\tilde{\nu}$ is limited by the size of the mesh cell. The implementation, based on the IDDES method (see Ref. 1), has been adjusted to comply with residual-based LES models. $\tilde{S}$, in the Spalart–Allmaras equation (Equation 3-169), is modified as

$$\tilde{S} = S + \frac{\tilde{\nu} f_{v2}}{\kappa_v^2 l_w^2} \tag{3-279}$$

and

$$l_w = \max\{f_d(1 + f_{restore})D_w, \min(D_w, 0.01266 C_{DES} h)\} \tag{3-280}$$

where D_w is the distance to the closest wall and h is the length of the longest edge of the mesh element. The function f_d is defined as

$$f_d = \max\{\tanh[(8r_{dt})^3], f_{step}\} \tag{3-281}$$

The first argument is nonzero inside attached turbulent boundary layers. The function f_{step} depends on the distance to the closest wall, and h as

$$f_{step} = \min(2e^{-9\alpha^2}, 1), \quad \alpha = 0.25 - \frac{D_w}{C_{DES} h} \tag{3-282}$$

f_{step} is 1 for $D_w < 0.5275 C_{DES} h$ and sharply approaches 0 away from the wall. At $D_w = C_{DES} h$, $f_{step} = 0.01266$. The function $f_{restore}$ is only nonzero in the region $0 < D_w < 0.5275 C_{DES} h$, and is added to amplify the RANS length scale, and thereby the turbulent viscosity, outside the viscous sublayer and the log layer. It is defined as

$$f_{restore} = \max(f_{hill} - 1, 0)\Psi f_{amp} \tag{3-283}$$

where

$$f_{\text{hill}} = \begin{cases} 2e^{-11.09\alpha^2}, & \alpha \geq 0 \\ 2e^{-9\alpha^2}, & \alpha < 0 \end{cases} \tag{3-284}$$

The amplification factor Ψ is purely empirical and is expressed in terms of the Spalart–Allmaras parameters

$$\Psi = \sqrt{\min\left\{100, \frac{1}{f_{\text{v1}}}\left(1 - \frac{f_{\text{v2}} c_{\text{b1}}}{f_{\text{w}}^{*} c_{\text{w1}} \kappa_{\text{v}}^2}\right)\right\}} \tag{3-285}$$

and

$$f_{\text{amp}} = 1 - \max\{\tanh([c_{\text{dt}}^2 r_{\text{dt}}]^3), \tanh([c_{\text{dl}}^2 r_{\text{dl}}]^{10})\} \tag{3-286}$$

where

$$r_{\text{dt}} = \frac{\nu_{\text{T}}}{S_1(\kappa_{\text{v}} D_{\text{w}})^2}, \quad r_{\text{dl}} = \frac{\nu}{S_1(\kappa_{\text{v}} D_{\text{w}})^2}, \quad \text{and } S_1 = \sqrt{\frac{\partial u_{\text{i}}}{\partial x_{\text{j}}}\frac{\partial u_{\text{i}}}{\partial x_{\text{j}}}} \tag{3-287}$$

with the parameters

$$f_{\text{w}}^{*} = 0.4241, \quad c_{\text{dt}} = 1.63, \quad c_{\text{dl}} = 3.55 \tag{3-288}$$

Inspecting Equation 3-280 and Equation 3-281, it can be seen that for $D_{\text{w}} < 0.5275 C_{\text{DES}} h$, the DES model operates in RANS mode with an amplified turbulent viscosity within regions outside the viscous sublayer and the log layer (determined by the function f_{amp}). For $D_{\text{w}} > 0.5275 C_{\text{DES}} h$, the DES model operates in DDES (Delayed Detached Eddy Simulation) mode inside attached turbulent boundary layers (determined by the first argument in Equation 3-281), or smoothly approaches the LES mode of operation away from the wall. The extent of the inner, "protected" RANS region can be controlled by changing the value of the C_{DES} parameter.

Reference for DES

1. M. Shur, P. Spalart, M. Stretlets, and A. Travin, "A hybrid RANS-LES approach with delayed DES and wall-modeled LES capabilities," *Int. J. Heat Fluid Flow*, vol. 29, no. 6, pp. 1638–1649, 2008.

Theory for the Rotating Machinery Interfaces

The theory for the Rotating Machinery, Laminar Flow and Rotating Machinery, Turbulent Flow interfaces is described in this section:

- About Rotating Machinery
- Frozen Rotor
- Setting Up a Rotating Machinery Model
- References

About Rotating Machinery

Both the Rotating Machinery, Laminar Flow and Rotating Machinery, Turbulent Flow interfaces model flow in geometries with rotating parts. For example, stirred tanks, mixers, and pumps.

The Navier–Stokes equations formulated in a rotating coordinate system read (Ref. 1 and Ref. 2)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{3-289}$$

$$\begin{gathered} \rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \nabla)\mathbf{v} + 2\rho\Omega \times \mathbf{v} = \\ \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} - \rho\left(\frac{\partial \Omega}{\partial t} \times \mathbf{r} + \Omega \times (\Omega \times \mathbf{r})\right) \end{gathered} \tag{3-290}$$

where $\mathbf{v}$ is the velocity vector in the rotating coordinate system, $\mathbf{r}$ is the position vector, and Ω is the angular velocity vector. The relation between $\mathbf{v}$ and the velocity vector in the stationary coordinate system is

$$\mathbf{u} = \mathbf{v} + \frac{\partial \mathbf{r}}{\partial t}$$

The Rotating Machinery, Fluid Flow interfaces solve Equation 3-289 and Equation 3-290, but reformulated in terms of a nonrotating coordinate system; that is, they solve for $\mathbf{u}$. This is achieved by invoking the Arbitrary Lagrangian–Eulerian Formulation

(ALE) machinery. In rotating domains, $\mathbf{x} = \mathbf{x}(\Omega, t)$ as prescribed in the Rotating Domain under Definitions. The Navier–Stokes equations on rotating domains then read

$$\frac{\partial \rho}{\partial T} - \frac{\partial \mathbf{x}}{\partial T} \cdot \nabla \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-291}$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial T} - \frac{\partial \mathbf{x}}{\partial T} \cdot \nabla \mathbf{u}\right) + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} \tag{3-292}$$

The derivative operator $\partial\rho/\partial T$ is the mesh time derivative of the density and appears in the equation view as `d(rmspf.rho,TIME)`. Analogously, $\partial \mathbf{U}/\partial T$ is the mesh time derivative of the velocity. The variable `TIME` replaces t as the variable for time.

The user input for a rotating domain prescribes the angular frequency, w. To calculate Ω, the physics interfaces set up an ODE variable for the angular displacement ω. The equation for ω is

$$\frac{d\omega}{dt} = w \tag{3-293}$$

Ω, is defined as w times the normalized axis of rotation. In 2D, the axis of rotation is the z direction while it in 3D is specified in the Rotating Domain features. If the model contains several rotating domains, each domain has its own angular displacement ODE variable.

In nonrotating domains, the ordinary Navier–Stokes equations are solved. The rotating and fixed parts need to be coupled together by an identity pair, where a continuity boundary condition is applied.

Wall and Interior Wall boundary conditions apply in the rotating domain provided that the Translational velocity under Wall Movement uses the default Automatic from frame option.

Arbitrary Lagrangian–Eulerian Formulation (ALE) in the *COMSOL Multiphysics Reference Manual*

Frozen Rotor

Equation 3-291 through Equation 3-293 must be solved using a Time Dependent study. This can be computationally expensive. The Rotating Machinery, Fluid Flow

interfaces therefore support the so-called frozen rotor approach. The frozen rotor approach assumes that the flow in the rotating domain, expressed in the rotating coordinate system, is fully developed. Equation 3-289 then reduces to

$$\nabla \cdot (\rho \mathbf{v}) = 0 \tag{3-294}$$

and Equation 3-290 to

$$\begin{aligned} \rho(\mathbf{v} \cdot \nabla)\mathbf{v} + 2\rho\Omega \times \mathbf{v} = \\ \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} - \rho\Omega \times (\Omega \times \mathbf{r}) \end{aligned} \tag{3-295}$$

Frozen rotor is both a study type and an equation form. When solving a rotating machinery model using a Frozen Rotor study step, the Rotating Machinery, Fluid Flow interfaces effectively solve Equation 3-294 and Equation 3-295 in a "rotating" domain, but "rotating" domains do not rotate at all. Boundary conditions remain transformed as if the domains were rotating, but the domains remain fixed, or frozen, in position. As in the time-dependent case, the Rotating Machinery, Fluid Flow interfaces solve for the velocity vector in the stationary coordinate system, $\mathbf{u}$, rather than for $\mathbf{v}$; the relation between them is written as

$$\mathbf{v} = \mathbf{u} - \Omega \times \mathbf{r}$$

To make Equation 3-291 and Equation 3-292 equivalent to Equation 3-294 and Equation 3-295, the Frozen Rotor study step defines a parameter `TIME`, which by default is set to zero (`TIME` appears in the Parameters node under Global Definitions). Equation 3-293 is replaced by

$$\omega = w\mathrm{TIME}$$

Since `TIME` is a parameter and $\mathbf{x}$ is a function of `TIME`, $\partial\mathbf{x}/\partial T$ evaluates to its correct value. Finally, $\partial\rho/\partial T = 0$ and the mesh time derivative of the velocity is replaced by

$$\frac{\partial \mathbf{u}}{\partial T} = \Omega \times \mathbf{u}$$

In nonrotating domains, the ordinary, stationary Navier–Stokes equations are solved. The Frozen Rotor study step invokes a stationary solver to solve the resulting equation system.

The frozen rotor approach can in special cases give the same solution as solving Equation 3-291 through Equation 3-293 to steady state. This is the case if, for example, the whole geometry is rotating, or if the model is invariant with respect to

the position of the rotating domain relative to the nonrotating domain. The latter is the case for a fan placed in the middle of a straight, cylindrical duct.

In most cases, however, there is no steady-state solution to the rotating machinery problem. Only a pseudo-steady state where the solution varies periodically around some average solution. In those cases, the frozen rotor approach gives an approximate solution to the pseudo-steady state. The approximation depends on the position in which the rotor is frozen, and the method cannot capture transient effects (see Ref. 3 and Ref. 4). An estimate of the effect of the rotor position can be obtained by making a parametric sweep over `TIME`.

The frozen rotor approach is very useful for attaining initial values for time-dependent simulations. Starting from a frozen rotor solution, the pseudo-steady state can be reached within a few revolutions, while starting from $\mathbf{u} = \mathbf{0}$ can require tens of revolutions. See, for example, Ref. 5.

Only interfaces that explicitly support frozen rotors are included in a Frozen Rotor study step.

Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Setting Up a Rotating Machinery Model

The Rotating Machinery, Fluid Flow interfaces primarily handle two types of geometries with rotating parts.

The first type is where the whole geometry rotates. Typical examples are individual parts in turbomachinery and lab-on-a-chip devices. For such cases, the selection for the Rotating Domain under the Definitions node should be all domains in the geometry.

The other type is geometries where it is possible to divide the modeled device into rotationally invariant geometries. The operation can be, for example, to rotate an impeller in a baffled tank, as in Figure 3-9 where the impeller rotates from position 1 to 2.

The first step to set up these type of models is to divide the geometry into two parts, as shown in Step 1a. Draw the geometry using separate domains for fixed and rotating parts. If you intend to do a time-dependent simulation, activate the assembly (using an assembly instead of a union, see Geometry Modeling and CAD Tools in the *COMSOL*

Multiphysics Reference Manual) and create identity pairs, which makes it possible to treat the domains as separate parts in an assembly.

The second step is to remove the nonrotating domains from the Rotating Domain selection (Step 1b).

Once this is done, proceed to the usual steps of setting the fluid properties, boundary conditions. Apply a Flow Continuity to assembly pairs (Step 2a). Then mesh and solve the problem.

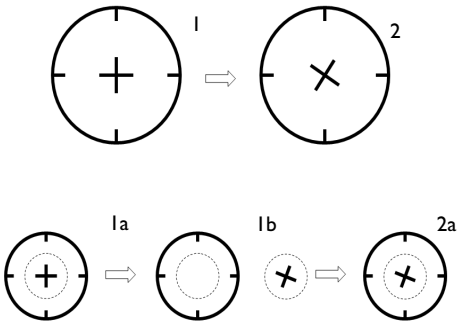

Figure 3-9: The modeling procedure in the Rotating Machinery, Fluid Flow interface.

References

1. H.P. Greenspan, *The Theory of Rotating Fluids*, Breukelen Press, 1990.

2. G.K. Batchelor, *An Introduction to Fluid Dynamics*, Cambridge University Press, 2000.

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4. A. Brucato, M. Ciofalo, F. Grisafi, and G. Micale, "Numerical Prediction of Flow Fields in Baffled Stirred Vessels: A Comparison of Alternative Modelling Approaches", *Chemical Engineering Science*, vol. 53, no. 21, pp. 3653–3684, 1998.

5. J.-P. Torré, D.F. Fletcher, T. Lasuye, and C. Xuereb, "Single and Multiphase CFD Approaches for Modelling Partially Baffled Stirred Vessels: Comparison of Experimental Data with Numerical Predictions", *Chemical Engineering Science*, vol. 62, no. 22, pp. 6246–6262, 2007.

Theory for the Viscoelastic Flow Interface

The theory for the Viscoelastic Flow interface is described in this section:

- General Viscoelastic Flow Theory
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- References for the Single-Phase Flow, Laminar Flow Interfaces

General Viscoelastic Flow Theory

The Viscoelastic Flow Interface is used to simulate incompressible and isothermal flow of viscoelastic fluids. It solves the continuity equation, the momentum balance equation, and a constitutive equation that defines the extra elastic stress contribution. The continuity and momentum balance can be expressed as

$$\rho\nabla\cdot\mathbf{u} = 0 \tag{3-296}$$

$$\rho\frac{\partial\mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\tau]+\mathbf{F} \tag{3-297}$$

where τ is the extra stress tensor, which is defined as a sum of a viscous and a viscoelastic or elastic contribution as

$$\tau = 2\mu_s\mathbf{S}+\mathbf{T}_e \tag{3-298}$$

where μ_s is the solvent viscosity, $\mathbf{S}$ is the strain-rate tensor, and $\mathbf{T}_e$ is the elastic (or viscoelastic) stress tensor. To adequately describe a flow of fluid with a complex rheological behavior, the symmetric stress tensor $\mathbf{T}_e$ is represented as a sum of the individual modes:

$$\mathbf{T}_e = \sum_m \mathbf{T}_{em} \tag{3-299}$$

To close the equation system, the constitutive relation for each mode is required.

The constitutive relation can be formulated using different dependent variables. Several commonly used constitutive models can be written using stress formulation as a hyperbolic partial differential transport equation of the form

$$\frac{1}{2\mu_{em}}\mathbf{f}_{rm}(\mathbf{T}_{em}) + \frac{\lambda_{em}}{2\mu_{em}}\overset{\nabla}{\mathbf{T}}_{em} = f_{pm}(\mathbf{T}_{em})\mathbf{S} \tag{3-300}$$

where the relaxation function $\mathbf{f}_{rm}$ and the viscosity factor f_{pm} are model-specific functions of stress, λ_{em} is a relaxation time, μ_{em} is a polymer viscosity, and the upper convective derivative operator is defined as

$$\overset{\nabla}{\mathbf{T}} \equiv \frac{\partial \mathbf{T}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{T} - [(\nabla\mathbf{u})\mathbf{T} + \mathbf{T}(\nabla\mathbf{u})^T] \tag{3-301}$$

The first two terms on the right-hand side represent the material derivative, and the other two terms represent the deformation. For more information, see Ref. 1.

OLDROYD-B MODEL

For the Oldroyd B model, the relaxation function and the viscosity factor are given by

$$\mathbf{f}_{rm} = \mathbf{T}_{em}, \qquad f_{pm} = 1 \tag{3-302}$$

The Oldroyd-B model can be derived from the kinetic theory representing the polymer molecules as suspensions of the Hookean spring in a Newtonian solvent. While demonstrating some basic features of viscoelasticity, the model can only predict a constant shear viscosity and gives unrealistic results for purely extensional flows due to the lack of a mechanism that limits the extensibility.

FENE-P MODEL

The finitely extensible nonlinear elastic model (FENE) is based on the kinetic theory that describes the polymer chains as a bead-spring dumbbell and accounts for finite extension of the polymer molecules. The FENE model with Peterlin closure (FENE-P) shows a finite extensibility and a shear-thinning behavior. The expressions for the relaxation function and the viscosity factor are given by

$$\mathbf{f}_{rm} = \left[1 + \frac{1}{L_{em}^2}\left(\frac{3}{1 - 3/L_{em}^2} + \frac{\lambda_{em}}{\mu_{em}}\mathrm{tr}(\mathbf{T}_{em})\right)\right]\mathbf{T}_{em}, \qquad f_{pm} = \frac{1}{1 - 3/L_{em}^2} \tag{3-303}$$

where L_{em} is the extensibility.

GIESEKUS MODEL

The Giesekus model is often used to model the flow of the semi-diluted and concentrated polymers. It adds the quadratic nonlinearity that is attributed to the effect of the hydrodynamic drag induced by the polymer-polymer interactions. The corresponding relaxation function and the viscosity factor are given by

$$\mathbf{f}_{r\mathrm{m}} = \left(1 + \alpha_{\mathrm{em}} \frac{\lambda_{\mathrm{em}}}{\mu_{\mathrm{em}}} \mathbf{T}_{\mathrm{em}}\right) \mathbf{T}_{\mathrm{em}}, \qquad f_{p\mathrm{m}} = 1 \tag{3-304}$$

where α_{em} is the dimensionless mobility factor.

BOUNDARY CONDITIONS

The theory about boundary conditions is found in the section Theory for the Single-Phase Flow Interfaces. Note that for the viscoelastic models, the extra stress tensor is defined as a sum of a viscous and an elastic contribution: $\tau = \mathbf{K} + \mathbf{T}_{\mathrm{e}}$. Therefore, an additional term should be added to the expression for the normal extra stress: $\mathbf{K}_{\mathrm{n}} = \mathbf{K}\mathbf{n} + \mathbf{T}_{\mathrm{e}}\mathbf{n}$.

Numerical Stability — Stabilization Techniques for Fluid Flow

The constitutive equations (Equation 3-300) can easily become unstable if discretized using the Galerkin finite element method (Ref. 2). Stabilized finite element methods are usually necessary in order to obtain physical solutions. The streamline diffusion method is used for the equations for the elastic stress tensor.

The theory about stabilization of the momentum equations Equation 3-296–Equation 3-297 is found in Numerical Stability — Stabilization Techniques for Fluid Flow.

Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*.

Solvers for Viscoelastic Flow

The default solver suggestions for single phase flow interfaces are discussed in Solvers for Laminar Flow. Note that if an iterative solver is used, the separate hybrid preconditioners are used for the velocity group and the viscoelastic stresses.

In the *COMSOL Multiphysics Reference Manual:*

- Selecting a Preconditioner for an Iterative Linear System Solver

Pseudo Time Stepping for Viscoelastic Flow Models

A stationary formulation has per definition no time derivatives. Solving Equation 3-296 through Equation 3-300 requires a starting guess that is close enough to the final solution. If no such guess is at hand, the fully transient problem can be solved instead. This is, however, a rather costly approach in terms of computational time. An intermediate approach is to add a fictitious time derivative. Further details is found in Pseudo Time Stepping for Laminar Flow Models.

References for the Viscoelastic Flow Interfaces

1. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, 2005.

2. T.J. Craven, J.M. Rees, and W.B. Zimmerman, "Stabilized finite element modelling of Oldroyd-B viscoelastic flow," *COMSOL Conference 2006*, Birmingham, U.K., 2006.

3. M.A. Alves, P.J.Oliveira, F.T. Pinho, "Numerical Methods for Viscoelastic Fluid Flows", *Annu. Rev. Fluid Mech.*, vol. 53, pp. 509-541, 2021

Theory for the Incompressible Potential Flow Interface

The theory for the Incompressible Potential Flow interface is described in the following section.

General Incompressible Potential Flow Theory

The Incompressible Potential Flow interface is used to simulate irrotational, inviscid, and incompressible flow. The continuity equation for incompressible flow can be expressed as a divergence-free constraint for the velocity

$$\nabla \cdot \mathbf{u} = 0 \tag{3-305}$$

Moreover, irrotational flow is described as

$$\nabla \times \mathbf{u} = 0 \tag{3-306}$$

As the curl of the gradient of a scalar field is zero by definition, the velocity can be approximated as the gradient of a scalar velocity potential, ϕ,

$$\mathbf{u} = -\nabla\phi \tag{3-307}$$

so that Equation 3-305 and Equation 3-307 result in the Laplace equation

$$-\nabla \cdot \nabla\phi = 0 \tag{3-308}$$

The local gauge pressure can be obtained from Bernoulli's equation

$$p = p_{\mathrm{Tot}} - \frac{\rho}{2}\|\nabla\phi\|^2 \tag{3-309}$$

where

$$p_{\mathrm{Tot}} = \frac{\rho}{2}U_{\mathrm{scale}}^2 \tag{3-310}$$

and U_{scale} is the user-defined free-stream velocity.

4

Heat Transfer and Nonisothermal Flow Interfaces

There are several physics interfaces included in the CFD Module to model heat transfer and nonisothermal flow. This chapter describes the physics interfaces found under the **Heat Transfer** branch ( ) as well as those under the **Fluid Flow** > **Nonisothermal Flow** branch ( ). The Modeling Heat Transfer in the CFD Module section helps you choose the best physics interface to start with.

- Modeling Heat Transfer in the CFD Module
- The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces
- The Rotating Machinery, Nonisothermal Flow Interface
- Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces
- Theory for the Nonisothermal Viscoelastic Flow

The documentation of all features in the Heat Transfer in Porous Media interface is now found in the *Heat Transfer Module User's Guide*, specifically in the following sections:

- The Heat Transfer Module Interfaces
- The Heat Transfer in Porous Media Interface

- Theory for the Heat Transfer Module
- Theory for Heat Transfer in Porous Media

Modeling Heat Transfer in the CFD Module

Heat transfer is an important phenomenon in many industrial processes. Often, a fluid plays a major role in transporting the heat and a detailed description of the flow field is necessary to accurately describe such processes. Typical examples are heating and cooling operations. Chemical reactions and phase changes are other commonly occurring phenomena. The temperature, in turn, affects the fluid properties and can alter the flow field. Natural convection is an example of this.

In this section:

- Selecting the Right Physics Interface
- Coupling to Other Physics Interfaces

Selecting the Right Physics Interface

The **Heat Transfer** branch ( ) included with this module has a number of physics interfaces that can be used to model energy transport. One or more of these can be added; either by themselves or together with other physics interfaces, typically flow physics interfaces.

While the standard COMSOL Multiphysics package includes physics interfaces for simulating heat transfer through conduction and convection, this module provides extra functionality within the standard Heat Transfer interfaces. The CFD Module also includes additional Heat Transfer interfaces such as The Heat Transfer in Porous Media Interface.

For heat transfer in single-phase flows, the CFD Module provides several turbulent (RANS) versions of the **Nonisothermal Flow** ( ) (located under the **Fluid Flow** branch) and **Conjugate Heat Transfer** ( ) (located under the **Heat Transfer** branch) multiphysics interfaces as well as three turbulent (LES) versions of the **Nonisothermal Flow** ( ) multiphysics interfaces, and the **Brinkman Equations** ( ) multiphysics interface, in addition to the laminar version available with the standard COMSOL Multiphysics package. The multiphysics interfaces automatically couple the flow and heat equations and they also provide functionality, such as support for turbulent heat transfer, that is not readily available when adding the interfaces separately.

HEAT TRANSFER IN SOLIDS OR FLUIDS, AND JOULE HEATING

The **Heat Transfer in Solids** ( ), **Heat Transfer in Fluids** ( ) (general convection and conduction), and **Electromagnetic Heating** > **Joule Heating** interfaces ( ), all belong to the COMSOL Multiphysics base package.

HEAT TRANSFER IN POROUS MEDIA

The **Heat Transfer in Porous Media** interface ( ) is an extension of the generic heat transfer interface that includes modeling heat transfer through convection, conduction, and radiation; conjugate heat transfer; and nonisothermal flow. The ability to define material properties, boundary conditions, and more for porous media heat transfer is also activated by selecting the **Heat transfer in porous media** checkbox on any heat transfer interface.

NONISOTHERMAL FLOW AND CONJUGATE HEAT TRANSFER

The **Nonisothermal Flow** ( ) and **Conjugate Heat Transfer** ( ) interfaces solve the Navier–Stokes equations together with an energy balance. They can also solve for heat transfer in solids.

Nonisothermal Flow and Conjugate Heat Transfer differ by their default features. The default heat transfer domain feature for Nonisothermal Flow is a Heat Transfer in Fluids node while Conjugate Heat Transfer has a Heat Transfer in Solids node as its default domain feature.

The Laminar Flow versions of the physics interfaces are used primarily to model slowly flowing fluids in environments where energy transport is also an important part of the system and application, and must be coupled or connected to the fluid flow in some way. Stokes' law (creeping flow) can be activated from the Nonisothermal Flow, Laminar Flow and Conjugate Heat Transfer, Laminar Flow interfaces if wanted. If you expect the flow to become turbulent, select one of the versions of the turbulent flow interfaces. Each physics interface includes a RANS or LES turbulence model to calculate the turbulence and algebraic models for the turbulent Prandtl number.

The Nonisothermal Flow and Conjugate Heat Transfer laminar and turbulent (RANS) flow interfaces can solve the fully compressible form of the Navier–Stokes equations. But boundary conditions and stabilizations are provided for Mach numbers less than

0.3. If you expect the Mach number in your model to become higher than 0.3, use The High Mach Number Flow Interfaces.

- Theory for the Heat Transfer Module in the *Heat Transfer Module User's Guide*
- The Joule Heating Interface in the *COMSOL Multiphysics Reference Manual*

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple heat transfer in turbulent flow to another type of phenomenon described by another physics interface. This can, for example, include chemical reactions and mass transport, as covered by the physics interfaces in the Chemical Species Transport branch.

Furthermore, the Chemical Reaction Engineering Module includes, not only support for setting up and simulating chemical reactions, but also for simulating reaction kinetics through the temperature-dependent Arrhenius Expression and Mass Action Law. This physics interface also includes support for including and calculating thermodynamic data as temperature-dependent expressions, for both reaction kinetics and fluid-flow.

In addition, if you also have the Heat Transfer Module, it includes more detailed descriptions and tools for simulating energy transport, such as surface-to-surface and participating media radiation.

Viscous Heating in a Fluid Damper: Application Library path **CFD_Module/Nonisothermal_Flow/fluid_damper**

A variety of modeling techniques are discussed in the following sections of the *Heat Transfer Module User's Guide*:

- Heat Transfer Variables
- Using the Boundary Conditions for the Heat Transfer Interfaces
- Handling Frames in Heat Transfer
- Heat Transfer and Fluid Flow Coupling
- Solver Settings

Also see The Heat Transfer Module Interfaces and Theory for the Heat Transfer Module.

The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces

In this section:

- Advantages of Using the Multiphysics Interfaces
- The Nonisothermal Flow, Laminar Flow and Turbulent Flow Interfaces
- The Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces
- The Nonisothermal Flow, Brinkman Equations Interface
- The Nonisothermal Flow, Viscoelastic Flow Interface
- Settings for Physics Interfaces and Coupling Features
- Coupling Feature
- Physics Interface Features
- Nonisothermal Flow
- Marangoni Effect

Advantages of Using the Multiphysics Interfaces

The Nonisothermal Flow and Conjugate Heat Transfer interfaces combine the heat equation with either laminar flow or turbulent flow and use either a **Heat Transfer in Fluids** or **Heat Transfer in Solids** domain model. The advantage of using the multiphysics interfaces is that predefined couplings are available in both directions. In particular, physics interfaces use the same definition of the density, which can therefore be a function of both pressure and temperature. Solving this coupled system of equations

usually requires numerical stabilization accounting for the couplings, which the predefined multiphysics interfaces also set up.

See also Heat Transfer and Fluid Flow Coupling in the *Heat Transfer Module User's Manual* for more information.

The Nonisothermal Flow, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the **Fluid Flow** > **Nonisothermal Flow** branch of the **Model Wizard** or **Add Physics** windows, one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) and **Heat Transfer** are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

- The **Laminar Flow** interface ( ) combines a Heat Transfer in Fluids interface with a Laminar Flow interface.
- The **Turbulent Flow, Algebraic yPlus** interface ( ) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface ( ) combines a Heat Transfer in Fluids interface with a Turbulent Flow, L-VEL interface.
- The **Turbulent Flow, k-ε** interface () combines a Heat Transfer in Fluids interface with a Turbulent Flow, k-ε interface.
- The **Turbulent Flow, Realizable k-ε** interface ( ) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Realizable k-ε interface.
- The **Turbulent Flow, k-ω** interface () combines a Heat Transfer in Fluids interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, SST** interface () combines a Heat Transfer in Fluids interface with a Turbulent Flow, SST interface.

- The **Turbulent Flow, Low Re k-ε** interface ( ) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, Spalart–Allmaras** interface ( ) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Spalart–Allmaras interface.
- The **Turbulent Flow, v2-f** interface ( ) combines a Heat Transfer in Fluids interface with a Turbulent Flow, v2-f interface.
- The **LES RBVM** interface ( ) combines a Heat Transfer in Fluids interface with an LES RBVM interface.
- The **LES RBVMWV** interface ( ) combines a Heat Transfer in Fluids interface with an LES RBVMWV interface.
- The **LES Smagorinsky** interface ( ) combines a Heat Transfer in Fluids interface with an LES Smagorinsky interface.

The Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the **Heat Transfer** > **Conjugate Heat Transfer** branch of the **Model Wizard** or **Add Physics** windows, **Heat Transfer** and one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

	The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

- The **Laminar Flow** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Laminar Flow interface.
- The **Turbulent Flow, Algebraic yPlus** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, L-VEL interface.
- The **Turbulent Flow, k-ε** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, k-ε interface.

- The **Turbulent Flow, Realizable k-ε** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, Realizable k-ε interface.
- The **Turbulent Flow, k-ω** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, Low Re k-ε** interface ( )combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, SST** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, SST interface.
- The **Turbulent Flow, Spalart–Allmaras** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, Spalart–Allmaras interface.
- The **Turbulent Flow, v2-f** interface ( ) combines a Heat Transfer in Solids and Fluids interface with a Turbulent Flow, v2-f interface.

The Nonisothermal Flow, Brinkman Equations Interface

When the **Brinkman Equations** multiphysics interface is added from the **Fluid Flow** > **Nonisothermal Flow** branch of the **Model Wizard** or **Add Physics** windows, the **Heat Transfer in Porous Media** and the **Brinkman Equations** interfaces are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

The Nonisothermal Flow, Viscoelastic Flow Interface

When the **Viscoelastic Flow** multiphysics interface ( ) is added from the **Fluid Flow** > **Nonisothermal Flow** branch of the **Model Wizard** or **Add Physics** windows, the **Heat Transfer in Fluids** and the **Viscoelastic Flow** interfaces are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

Settings for Physics Interfaces and Coupling Features

When physics interfaces are added using the predefined couplings, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings may not be automatically included.

For example, if single Heat Transfer in Fluids and Laminar Flow interfaces are added, COMSOL Multiphysics adds an empty **Multiphysics** node. When you right-click this node, you can add the **Nonisothermal Flow** coupling feature, but the modified settings are not included. To get all the modified settings presented below automatically, you may instead right-click the component node, select **Add Multiphysics**, and add the **Nonisothermal Flow** coupling feature from the **Add Multiphysics** window.

TABLE 4-1: MODIFIED SETTINGS FOR THE NONISOTHERMAL FLOW INTERFACES.

PHYSICS OR COUPLING INTERFACE	MODIFIED SETTINGS (IF ANY)
Heat Transfer in Solids	Discretization order from temperature Lagrange shape function is 1. A **Heat Transfer in Fluids** feature is added with a default editable selection set to **All domains**. The **Absolute pressure**, p_A (**Model Input** section) and the **Velocity field**, $\mathbf{u}$ (**Heat Convection** section) are automatically set to the variables from the **Nonisothermal Flow** multiphysics coupling feature.
Heat Transfer in Fluids	The **Absolute pressure**, p_A (**Model Input** section) and the **Velocity field**, $\mathbf{u}$ (**Heat Convection** section) are automatically set to the variables from the **Nonisothermal Flow** multiphysics coupling feature.
Nonisothermal Flow	The fluid-flow and heat-transfer interfaces are preselected The **Compressibility** option of the fluid flow interface is set to **Weakly Compressible** for the laminar and turbulent (RANS) flow interfaces and to **Incompressible** for the LES interfaces.

Coupling Feature

The Nonisothermal Flow multiphysics coupling node is described in this section.

Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

HEAT TRANSFER IN FLUIDS (NONISOTHERMAL FLOW)

The available physics features for The Heat Transfer in Fluids Interface are listed in the section The Heat Transfer in Solids and Fluids Interface. Also see Fluid in the *Heat Transfer Module User's Guide* for details about that feature.

HEAT TRANSFER IN SOLIDS (CONJUGATE HEAT TRANSFER)

The available physics features for The Heat Transfer in Solids Interface are listed in the section The Heat Transfer in Fluids Interface. Also see Solid in the *Heat Transfer Module User's Guide* for details about that feature.

HEAT TRANSFER IN POROUS MEDIA

The available physics features for The Heat Transfer in Porous Media Interface are listed in the section The Heat Transfer in Porous Media Interface. Also see Porous Medium in the *Heat Transfer Module User's Guide* for details about that feature.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, ALGEBRAIC YPLUS

The available physics features for The Turbulent Flow, Algebraic yPlus Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, L-VEL

The available physics features for The Turbulent Flow, L-VEL Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ε

The available physics features for The Turbulent Flow, k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, REALIZABLE k-ε

The available physics features for The Turbulent Flow, Realizable k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ω

The available physics features for The Turbulent Flow, k-ω Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE k-ε

The available physics features for The Turbulent Flow, Low Re k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SPALART–ALLMARAS

The available physics features for The Turbulent Flow, Spalart–Allmaras Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, V2-F

The available physics features for The Turbulent Flow, v2-f Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LES RBVM

The available physics features for The LES RBVM Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LES RBVMWV

The available physics features for The LES RBVMWV Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LES SMAGORINSKY

The available physics features for The LES Smagorinsky Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

BRINKMAN EQUATIONS

The available physics features for The Brinkman Equations Interface are listed in the section Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface.

VISCOELASTIC FLOW

The available physics features for The Viscoelastic Flow Interface are listed in the section Domain, Boundary, Point, and Pair Nodes for the Viscoelastic Interface.

Nonisothermal Flow

Use the **Nonisothermal Flow** ( ) multiphysics coupling to simulate fluid flows where the fluid properties depend on temperature. Models can also include heat transfer in solids or in porous media as well as surface-to-surface radiation and radiation in participating media, with the Heat Transfer Module. The laminar and turbulent (RANS-EVM, RANS-RSM or LES) physics interfaces support low Mach numbers (typically less than 0.3). The Viscoelastic Flow interface only supports incompressible flow.

The **Nonisothermal Flow** multiphysics interfaces solve for conservation of energy, mass, and momentum in fluids and porous media and for conservation of energy in solids.

It defines p and $\mathbf{u}$ variables in order to set the **Absolute pressure** in the **Model Input** section and the **Velocity field** in the **Heat Convection** section of the **Fluid** feature and subfeature, in the Heat Transfer interface. In addition it provides all the fluids quantities that may be needed by the Heat Transfer interface (for example, viscosity, turbulence parameters).

In the Fluid Flow interface, it sets the **Temperature** in the **Model Input** section and defines the **Density** in the **Fluid Properties** section of the **Fluid Properties** and **Fluid and Matrix Properties** features.

It synchronizes also the definition of the reference temperature to be used for incompressible flows, and the features from the **Heat Transfer** and **Fluid Flow** interfaces when a turbulent flow regime is defined. It also complements the **Screen** and **Interior Fan** feature from the flow interface to account for thermal effects.

In addition, it also accounts for the multiphysics stabilization terms, for the heat transfer changes in the turbulent regime (for example, thermal wall functions), for work due to pressure forces and viscous dissipation, and for natural convection, including a Boussinesq approximation.

Nonisothermal Flow and **Conjugate Heat Transfer** trigger pseudo time stepping when **Use pseudo time stepping for stationary equation form** in the **Fluid Flow** interface is set to **Automatic from physics**.

The multiphysics stabilizations (streamline diffusion and crosswind diffusion) are controlled by the Fluid Flow interface. For example, the multiphysics streamline diffusion can be disabled in a **Laminar Flow** physics node, in the **Stabilization** section. The stabilization selected in the Heat Transfer interface has no effect if the multiphysics coupling stabilization is active, but remains active if not. However, the isotropic diffusion is not a multiphysics stabilization and is controlled by each physics interface. The crosswind diffusion stabilization is turned off for the LES interfaces.

Finally, when one of the physics interfaces or the multiphysics coupling is not solved in a study step, then the stabilization of each solved physics is used instead of the coupled stabilization, and the solver suggestions are uncoupled.

The pressure, velocity, and temperature variables of the **Nonisothermal Flow** coupling node are set to the **Common Model Input** values of the **Default Model Inputs** node on its complementary selection, that is, all domains except those from the **Selection** list. It allows to couple multiple fluid flow interfaces with a single heat transfer interface. See Default Model Inputs in the *COMSOL Multiphysics Reference Manual* for details.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `nitf1`.

DOMAIN SELECTION

The **Nonisothermal Flow** coupling node selection is locked to the union of:

- The intersection of the **Fluid** or **Moist Air** feature's selection with the **Fluid Properties** feature's selection.
- The intersection of the **Fluid** feature's selection within the Heat Transfer in Fluids interface and the **Fluid Properties** feature's selection within the Viscoelastic Flow interface.
- The intersection of the **Porous Medium** feature's selection within the Heat Transfer in Porous Media interface and the **Porous Medium** feature's selection within the Brinkman Equations interface.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Heat transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created:

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Heat Transfer in Fluids** is deleted, then the **Heat transfer** list defaults to **None** as there is nothing to couple to.

HEAT TRANSFER TURBULENCE MODEL

This section is available when the fluid flow interface uses a turbulence model. When a RANS turbulence model is used, select an option from the **Heat transport turbulence model** list: **Kays–Crawford** (the default), **Extended Kays–Crawford**, or **User-defined turbulent Prandtl number**.

For **Extended Kays–Crawford**, enter a **Reynolds number at infinity** $\mathrm{Re}_{\mathrm{inf}}$ (dimensionless).

For **User-defined turbulent Prandtl number**, enter a **Turbulent Prandtl number** Pr_{T} (dimensionless).

When the flow interface uses a RANS turbulence model, the conductive heat flux is defined as

$$q = -(k + k_{\mathrm{T}})\nabla T$$

with the turbulent thermal conductivity defined as

$$k_{\mathrm{T}} = \frac{\mu_{\mathrm{T}} C_p}{\mathrm{Pr}_{\mathrm{T}}}$$

where μ_{T} is defined by the flow interface, and Pr_{T} depends on the **Heat transport turbulence model**. See Turbulent Conductivity for details.

This section is also available when either of the LES interfaces RBVMWV or Smagorinsky is used. For these two LES models, additional diffusion terms, corresponding to the ones in the momentum equation, appear in the energy equation. The magnitude of these terms can be controlled by a turbulent Prandtl number.

The **Turbulence model type** used by the fluid flow interface can be displayed by selecting the **Show or Hide Physics Property Settings** button at the right of the **Fluid flow** list.

When the **Wall treatment** option selected in the fluid flow interface is set either to **Wall functions** or **Automatic**, the **Thermal wall function** can be set to **Standard** (default) or **High viscous dissipation at wall**. The **Standard** option is suitable for most of the configurations. The **High viscous dissipation at wall** option accounts for viscous dissipation in the boundary layer which is not the case with the **Standard** option. This is needed for accurate results in case of fast internal flow, especially if paths are narrow or the fluid very viscous. See Temperature Condition for Automatic Wall Treatment and Wall functions for details.

MATERIAL PROPERTIES

Boussinesq Approximation

When the **Compressibility** setting in the fluid flow interface is set to **Incompressible**, select the **Boussinesq approximation** checkbox in order to use material data evaluated at the reference temperature and reference pressure. If gravity is included in the physics, it is linearized with respect to temperature.

Density

Select an option from the **Specify density** list: **From heat transfer interface** (the default), **From fluid flow interface**, **Custom, linearized density**, or **Custom**:

- For **From heat transfer interface**: define the **Density** ρ in the **Thermodynamics, Fluid** section of the **Fluid** node, in the Heat Transfer coupled interface. Depending on the **Fluid type** option in this node, the density may bet taken from material, set directly, or computed by using the ideal gas law. The same value is automatically set in the **Fluid Properties** section of the **Fluid Properties** node, in the Fluid Flow coupled interface.
- For **From fluid flow interface**: define the **Density** ρ in the **Fluid Properties** section of the **Fluid Properties** node, in the Fluid Flow coupled interface. The same value is automatically set in the **Thermodynamics, Fluid** section of the **Fluid** node, in the Heat Transfer coupled interface.
- For **Custom, linearized density**, enter the **Reference density** ρ_{ref} (SI unit: kg/m^3) and the **Coefficient of thermal expansion** α_p (SI unit: $1/\text{K}$), or select **From material**, or select a variable in the list if available. Regardless how the properties are defined they should be constant. If material properties are not constant you should consider using any of the other options to define the density. Also, if **Custom, linearized density** is used for incompressible flow, the density ρ is evaluated to ρ_{ref}. In this case α_p is not used unless **Boussinesq approximation** is selected. The same value is automatically set in the **Fluid Properties** section of the **Fluid Properties** node, in the Fluid Flow coupled interface, and in the **Thermodynamics, Fluid** section of the **Fluid** node, in the Heat Transfer coupled interface.
- For **Custom**, enter a **Density** ρ (SI unit: kg/m^3), or select a density in the list if available. The same value is automatically set in the **Fluid Properties** section of the **Fluid Properties** node, in the Fluid Flow coupled interface, and in the **Thermodynamics, Fluid** section of the **Fluid** node, in the Heat Transfer coupled interface.

See Fluid Properties and Fluid in the *COMSOL Multiphysics Reference Manual* for details.

When the coupled heat transfer interface is also coupled to a phase transport interface via the Nonisothermal Mixture Model multiphysics coupling, **Specify density** must be set to **From fluid flow interface**.

The density definition in the **Nonisothermal Flow** node ensures that the same definition of the density is used on the fluid flow and heat transfer interfaces. When **Include gravity** is selected and the **Compressibility** is set to **Incompressible flow** in the fluid interface properties, the gravity forces are defined using the coefficient of thermal expansion. Along with the fact that the material properties are evaluated for a constant temperature and pressure, this gravity force definition corresponds to Boussinesq approximation. Unless the density is defined as **Custom, linearized density** the coefficient of thermal expansion is evaluated from the fluid density.

Reference Temperature

Select an option from the **Specify reference temperature** list — **From heat transfer interface**, **From fluid flow interface** (the default), or **User defined**.

For **From heat transfer interface**, set the **Reference temperature** T_{ref} (SI unit: K) in the **Physical Model** section of the interface selected in the **Heat transfer** list of the **Coupled Interfaces** section. The **Reference temperature** input in the **Fluid flow** interface is synchronized to the same value or expression, and is not editable.

For **From fluid flow interface**, set the **Reference temperature** T_{ref} (SI unit: K) in the **Physical Model** section of the interface selected in the **Fluid flow** list of the **Coupled Interfaces** section. The **Reference temperature** input in the **Heat transfer** interface is synchronized to the same value or expression, and is not editable.

For **User defined**, set a value or expression. The **Reference temperature** inputs in the **Physical Model** sections of the **Heat transfer** and **Fluid flow** interfaces are synchronized to the same value or expression, and are not editable.

When the coupled heat transfer interface is also coupled to a phase transport interface via the Nonisothermal Mixture Model multiphysics coupling, **Specify reference temperature** must be set to **From fluid flow interface**.

ENERGY BALANCE

The **Include viscous dissipation** checkbox is selected by default to account for the heat source corresponding to viscous heating. Because it may induce an extra computational cost it should be only selected in application where such effect is expected. If no information on this is available, selecting the option ensures that the energy balance for the heat and the flow equation is respected.

When the **Include kinetic energy** checkbox is selected, the conservative total-energy equation is solved. Because this option may induce an extra computational cost, it is only selected by default for weakly compressible and compressible LES.

If the coupled interface is Viscoelastic Flow, the **Include irreversible losses** checkbox is available. The checkbox is selected by default to account for the heat source corresponding to the heating due to irreversible losses.

When an interface is selected from the **Heat transfer** list, some of its model inputs are forced with values from the **Nonisothermal Flow** node. In addition, it defines how the turbulence has to be accounted for, depending on the **Fluid flow** interface's turbulence settings.

Therefore, each fluid flow interface should be used in at most one **Nonisothermal Flow** node. In cases where multiple fluid flow interfaces are used, they can be coupled with a single heat transfer interface, using an equal number of **Nonisothermal Flow** nodes to define proper multiphysics couplings. In the **Heat transfer** interface, the inputs for pressure and velocity are then taken from the first **Nonisothermal Flow** node.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Heat transfer** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

See also Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces in the *CFD Module User's Manual* for more information.

See also Theory for the Nonisothermal Viscoelastic Flow in the *CFD Module User's Manual* for more information.

Marangoni Effect

The **Marangoni Effect** multiphysics coupling ( ) accounts for Marangoni convection. Marangoni convection occurs when the surface tension of a fluid-fluid interface (generally liquid-air) depends on the concentration of a species or on the temperature distribution. In the case of temperature dependence, the Marangoni effect is also called thermo-capillary convection. It is of primary importance in the fields of welding, crystal growth, and electron beam melting of metals.

The Marangoni effect is a shear stress that depends on the tangential and normal variations of surface tension with temperature gradient. It has the following contribution described by forces induced on the fluid/fluid interface:

$$\left[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right]\mathbf{n}\;=\;\sigma(\nabla_{\mathrm{t}}\cdot\mathbf{n})\mathbf{n}-\nabla_{\mathbf{t}}\sigma$$

where σ is the surface tension coefficient (N/m). The first term on the right-hand-side accounts for the normal forces related to curvature effects, while the second term stands for tangential forces. Note that this formulation is intended for laminar flow regimes only.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `mar1`.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Heat transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder** — for example, **Heat Transfer in Fluids** is deleted — then the **Heat transfer** list defaults to **None** as there is nothing to couple to.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Heat transfer** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

SURFACE TENSION

Select a **Surface tension coefficient type**: **Library coefficient, liquid/gas interface** or **User defined** (the default).

- For **Library coefficient, liquid/gas interface** choose an option from the **Library surface tension coefficient** list.
- For **User defined** enter a **Surface tension coefficient** σ (SI unit: N/m).

CONTACT ANGLE

The attachment angle between the fluid/fluid interface and the adjacent walls can be specified in this section.

Select an option from the **Specify contact angle** list — **Directly** (the default) or **Through Young's equation**.

- For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians.
- For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

The Rotating Machinery, Nonisothermal Flow Interface

In this section:

- Rotating Machinery, Nonisothermal Flow, Laminar Flow Interface
- Domain, Boundary, Edge, Point, and Pair Nodes for the Rotating Machinery, Nonisothermal Flow Interfaces

Rotating Machinery, Nonisothermal Flow, Laminar Flow Interface

The **Laminar Flow** version of the **Rotating Machinery, Nonisothermal Flow** multiphysics interface ( ), found under the **Fluid Flow** > **Nonisothermal Flow** > **Rotating Machinery, Nonisothermal Flow** branch ( ) when adding a physics interface, is used to simulate laminar flow and heat transfer in equipment containing one or more rotating parts.

This physics interface combines the capabilities of the Rotating Machinery, Laminar Flow interface and the Heat Transfer in Fluids interface, and can be used to simulate fluid flows where the fluid properties depend on the temperature. Furthermore it is also possible to include heat transfer in solids, stationary and rotating, as well as surface-to-surface radiation and radiation in participating media. The physics interface is available in 2D and 3D and supports low Mach number (typically less than 0.3) flows, as well as non-Newtonian fluids.

Four study types are available for this physics interface. Using the **Time Dependent** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. The **Time Dependent, One-Way NITF** and **Frozen Rotor, One-Way NITF** study are used for frozen rotor and time dependent nonisothermal flow computations where the temperature variations are so small that they do not affect the flow.

When adding the multiphysics interface, the **Laminar Flow** and **Heat Transfer in Fluids** interfaces are added to the Model Builder. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** node. In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**. The following default nodes are also added in the

Model Builder under **Laminar Flow** — **Fluid Properties**, **Wall,** and **Initial Values**; and under **Heat Transfer in Fluids** — **Fluid**, **Thermal Insulation**, and **Initial Values**.

In earlier versions of COMSOL Multiphysics (prior to version 5.4), a specific physics interface called **Rotating Machinery, Nonisothermal Flow (rmnitf)** was added to the **Model Builder**. Now, a predefined multiphysics coupling approach is used, improving the flexibility and design options for your modeling. For specific details, see The Multiphysics Branch and Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual.*

- Domain, Boundary, Edge, Point, and Pair Nodes for the Rotating Machinery, Nonisothermal Flow Interfaces
- Theory for the Free Surface Features in the *Mixer Module User's Guide*
- Modeling Heat Transfer in the CFD Module
- The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces
- Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

The **Time Dependent, One-Way NITF** and **Frozen Rotor, One-Way NITF** studies are used for frozen rotor and time dependent nonisothermal flow computations where the temperature variations are so small that they do not affect the flow.

Domain, Boundary, Edge, Point, and Pair Nodes for the Rotating Machinery, Nonisothermal Flow Interfaces

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (macOS or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

HEAT TRANSFER IN FLUIDS (NONISOTHERMAL FLOW)

The available physics features for The Heat Transfer in Fluids Interface are listed in the section The Heat Transfer in Solids and Fluids Interface. Also see Fluid for details about that feature.

LAMINAR FLOW

The available physics features for The Rotating Machinery, Laminar Flow Interface are listed in the section Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

In this section:

- The Nonisothermal Flow and Conjugate Heat Transfer Equations
- Turbulent Nonisothermal Flow Theory
- The Boussinesq Approximation
- Theory for the Nonisothermal Screen Boundary Condition
- Theory for the Interior Fan Boundary Condition
- References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

The Nonisothermal Flow and Conjugate Heat Transfer Equations

In industrial applications it is common that the density of a process fluid varies. These variations can have a number of different sources, but the most common one is the presence of an inhomogeneous temperature field. This module includes the Nonisothermal Flow predefined multiphysics coupling to simulate systems in which the density varies with temperature.

Other situations where the density might vary includes chemical reactions (for instance, where reactants associate or dissociate).

The Nonisothermal Flow and Conjugate Heat Transfer interfaces contain the fully compressible formulation of the continuity and momentum equations:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \nabla \cdot \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) + \mathbf{F} \end{aligned} \tag{4-1}$$

where

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)

- p is the pressure (SI unit: Pa)
- μ is the dynamic viscosity (SI unit: Pa·s)
- $\mathbf{F}$ is the body force vector (SI unit: $\mathrm{N/m^3}$)

It also solves the heat equation, which for a fluid is given by

$$\rho C_p\left(\frac{\partial T}{\partial t}+(\mathbf{u}\cdot\nabla)T\right)=-(\nabla\cdot\mathbf{q})+\tau:\mathbf{S}-\frac{T}{\rho}\frac{\partial\rho}{\partial T}\bigg|_p\left(\frac{\partial p}{\partial t}+(\mathbf{u}\cdot\nabla)p\right)+Q \qquad (4\text{-}2)$$

where in addition to the quantities above

- C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- $\mathbf{q}$ is the heat flux by conduction (SI unit: $\mathrm{W/m^2}$)
- τ is the viscous stress tensor (SI unit: Pa)
- $\mathbf{S}$ is the strain-rate tensor (SI unit: 1/s)

$$\mathbf{S}=\frac{1}{2}(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)$$

- Q contains heat sources other than viscous heating (SI unit: $\mathrm{W/m^3}$)

The *work done by pressure changes* term

$$\alpha_p T\left(\frac{\partial p}{\partial t}+\mathbf{u}\cdot\nabla p\right) \text{ with } \alpha_p=-\frac{1}{\rho}\frac{\partial\rho}{\partial T}\bigg|_p .$$

and the *viscous heating* term

$$\tau:\mathbf{S}$$

are often negligible. The pressure work term is included by default, while the viscous heating term is optional. The latter can be accounted for by selecting the corresponding checkbox in the Nonisothermal Flow feature. When, in addition, the **Include kinetic energy** checkbox is selected, the conservative total-energy equation is solved

$$\frac{\partial}{\partial t}\left[\rho\left(e+\frac{1}{2}\|\mathbf{u}\|^2\right)\right]+\nabla\cdot\left[\rho\mathbf{u}\left(h+\frac{1}{2}\|\mathbf{u}\|^2\right)\right]=\nabla\cdot(\mathbf{u}\cdot\tau-\mathbf{q})+Q \qquad (4\text{-}3)$$

where

$$h = h(T_{\text{ref}}, p_{\text{ref}}) + \int_{T_{\text{ref}}}^{T} C_p dT + \int_{p_{\text{ref}}}^{p} \frac{(1 - \alpha_p T)}{\rho} dp, \quad e = h - \frac{p}{\rho} \tag{4-4}$$

Observe that the pressure in the pressure work term always is the absolute pressure even if a reduced pressure is used in the momentum equation. For a detailed discussion of the fundamentals of heat transfer in fluids, see Ref. 3.

The physics interface also supports heat transfer in solids:

$$\rho C_p \frac{\partial T}{\partial t} = -(\nabla \cdot \mathbf{q}) + Q + Q_{\text{ted}}$$

where Q_{ted} is the thermoelastic damping heat source (SI unit: $\text{W}/(\text{m}^3)$). This term is not included by default but must be added by selecting corresponding checkbox.

- Theory for Heat Transfer in Fluids in the *Heat Transfer Module User's Manual.*
- Turbulent Nonisothermal Flow Theory
- References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

Turbulent Nonisothermal Flow Theory

Turbulent energy transport is conceptually more complicated than energy transport in laminar flows since the turbulence is also a form of energy.

Equations for compressible turbulence are derived using the Favre average. The Favre average of a variable T is denoted $\tilde{T}$ and is defined by

$$\tilde{T} = \frac{\overline{\rho T}}{\bar{\rho}}$$

where the bar denotes the usual Reynolds average. The full field is then decomposed as

$$T = \tilde{T} + T''$$

With this notation the equation for total internal energy, e, becomes

$$\frac{\partial}{\partial t}\left(\bar{\rho}\left(\tilde{e}+\frac{\tilde{u}_i\tilde{u}_i}{2}\right)+\frac{\overline{\rho u_i''u_i''}}{2}\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\left(\tilde{h}+\frac{\tilde{u}_i\tilde{u}_i}{2}\right)+\tilde{u}_j\frac{\overline{\rho u_i''u_i''}}{2}\right)=$$
$$\frac{\partial}{\partial x_j}\left(-q_j-\overline{\rho u_j''h''}+\overline{\tau_{ij}u_i''}-\frac{\overline{\rho u_j''u_i''u_i''}}{2}\right)+\frac{\partial}{\partial x_j}(\tilde{u}_i(\overline{\tau_{ij}}-\overline{\rho u_i''u_j''})) \quad (4\text{-}5)$$

where h is the enthalpy. The vector

$$q_j = -\lambda\frac{\partial T}{\partial x_j} \quad (4\text{-}6)$$

is the laminar conductive heat flux and

$$\tau_{ij} = 2\mu S_{ij}-\frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}$$

is the laminar, viscous stress tensor. Notice that the thermal conductivity is denoted λ.

The modeling assumptions are in large part analogous to those for incompressible turbulence modeling. The stress tensor

$$-\overline{\rho u_i''u_j''}$$

is modeled using the *Boussinesq approximation*:

$$-\overline{\rho u_i''u_j''} = \bar{\rho}\tau^T{}_{ij} = 2\mu_T\left(\tilde{S}_{ij}-\frac{1}{3}\frac{\partial\tilde{u}_k}{\partial x_k}\delta_{ij}\right)-\frac{2}{3}\bar{\rho}k\delta_{ij} \quad (4\text{-}7)$$

where k is the turbulent kinetic energy, which in turn is defined by

$$\bar{\rho}k = \frac{1}{2}\overline{\rho u_i''u_i''} \quad (4\text{-}8)$$

The correlation between u_j'' and h'' in Equation 4-5 is the turbulent transport of heat. It is modeled analogously to the laminar conductive heat flux

$$\overline{\rho u_j''h''} = q^T{}_j = -\lambda_T\frac{\partial\tilde{T}}{\partial x_j} = -\frac{\mu_T C_p}{Pr_T}\frac{\partial\tilde{T}}{\partial x_j} \quad (4\text{-}9)$$

The molecular diffusion term

$$\overline{\tau_{ij}u_i''}$$

and the turbulent transport term

$$\overline{\rho u_j'' u_i'' u_i''}/2$$

are modeled by a generalization of the molecular diffusion and turbulent transport terms found in the incompressible k equation

$$\overline{\tau_{ij} u_i''} - \frac{\overline{\rho u_j'' u_i'' u_i''}}{2} = \left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j} \tag{4-10}$$

Inserting Equation 4-6 through Equation 4-10 into Equation 4-5 gives

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\bar{\rho}\left(\tilde{e} + \frac{\tilde{u}_i \tilde{u}_i}{2} + k\right)\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\left(\tilde{h} + \frac{\tilde{u}_i \tilde{u}_i}{2} + k\right)\right) = \\ &\frac{\partial}{\partial x_j}\left(-q_j - q^T{}_j + \left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\tilde{u}_i(\overline{\tau_{ij}} + \bar{\rho}\tau^T{}_{ij}))\end{aligned} \tag{4-11}$$

The Favre average can also be applied to the momentum equation, which, using Equation 4-7, can be written

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{u}_i) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} + \bar{\rho}\tau^T{}_{ij}) \tag{4-12}$$

Taking the inner product between $\tilde{u}_i$ and Equation 4-12 results in an equation for the resolved kinetic energy, which can be subtracted from Equation 4-11 with the following result:

$$\begin{aligned}&\frac{\partial}{\partial t}(\bar{\rho}(\tilde{e} + k)) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j(\tilde{e} + k)) = -\bar{p}\frac{\partial \tilde{u}_j}{\partial x_j} + \\ &\frac{\partial}{\partial x_j}\left(-q_j - q^T{}_j + \left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\tilde{u}_i(\overline{\tau_{ij}} + \bar{\rho}\tau^T{}_{ij}))\end{aligned} \tag{4-13}$$

where the relation

$$\tilde{h} = \tilde{e} + \bar{p}/\bar{\rho}$$

has been used.

According to Wilcox (Ref. 1), it is usually a good approximation to neglect the contributions of k for flows with Mach numbers up to the supersonic range. This gives the following approximation of Equation 4-13 is

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{e}) = -\bar{p}\frac{\partial \tilde{u}_j}{\partial x_j} + \frac{\partial}{\partial x_j}(-q_j - q^T{}_j) + \frac{\partial}{\partial x_j}(\tilde{u}_i(\overline{\tau_{ij}} + \bar{\rho}\tau^T{}_{ij})) \qquad (4\text{-}14)$$

Larsson (Ref. 2) suggests to make the split

$$\overline{\tau_{ij}} = \tilde{\tau}_{ij} + \overline{\tau_{ij}}''$$

Since

$$\tilde{\tau}_{ij} \gg \overline{\tau_{ij}}''$$

for all applications of engineering interest, it follows that

$$\overline{\tau_{ij}} \approx \tilde{\tau}_{ij}$$

and consequently

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{e}) = -\bar{p}\frac{\partial \tilde{u}_j}{\partial x_j} + \frac{\partial}{\partial x_j}\left((\lambda + \lambda_T)\frac{\partial \tilde{T}}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\tilde{u}_i\tilde{\tau}^{\mathrm{Tot}}_{ij}) \qquad (4\text{-}15)$$

where

$$\tilde{\tau}^{\mathrm{Tot}}_{ij} = (\mu + \mu_T)\left(2\tilde{S}_{ij} - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)$$

Equation 4-15 is completely analogous to the laminar energy equation and can be expanded using the same theory (see for example Ref. 3):

$$\bar{\rho}C_p\left(\frac{\partial \tilde{T}}{\partial t} + \tilde{u}_j\frac{\partial \tilde{T}}{\partial x_j}\right) = \frac{\partial}{\partial x_j}\left((\lambda + \lambda_T)\frac{\partial \tilde{T}}{\partial x_j}\right) + \tilde{\tau}_{ij}\tilde{S}_{ij} - \frac{\tilde{T}}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial \tilde{T}}\bigg|_{\bar{p}}\left(\frac{\partial \bar{p}}{\partial t} + \tilde{u}_j\frac{\partial \bar{p}}{\partial x_j}\right)$$

which is the temperature equation solved in the turbulent Nonisothermal Flow and Conjugate Heat Transfer interfaces.

TURBULENT CONDUCTIVITY

Kays–Crawford

This is a relatively exact model for Pr_T, while still quite simple. In Ref. 4, it is compared to other models for Pr_T and found to be a good approximation for most kinds of turbulent wall bounded flows except for turbulent flow of liquid metals. The model is given by

$$\mathrm{Pr}_T = \left(\frac{1}{2\mathrm{Pr}_{T\infty}} + \frac{0.3}{\sqrt{\mathrm{Pr}_{T\infty}}}\frac{C_p\mu_T}{\lambda} - \left(0.3\frac{C_p\mu_T}{\lambda}\right)^2\left(1 - e^{-\lambda/(0.3C_p\mu_T\sqrt{\mathrm{Pr}_{T\infty}})}\right)\right)^{-1} \quad (4\text{-}16)$$

where the Prandtl number at infinity is $\mathrm{Pr}_{T\infty} = 0.85$ and λ is the conductivity.

Extended Kays–Crawford

Weigand and others (Ref. 5) suggested an extension of Equation 4-16 to liquid metals by introducing

$$\mathrm{Pr}_{T\infty} = 0.85 + \frac{100\lambda}{C_p\mu\mathrm{Re}_\infty^{0.888}}$$

where Re_∞, the Reynolds number at infinity, must be provided either as a constant or as a function of the flow field. You enter the Reynolds number in the Model Inputs section of the Fluid feature.

TEMPERATURE CONDITION FOR AUTOMATIC WALL TREATMENT AND WALL FUNCTIONS

Both automatic wall treatment and wall functions introduce a theoretical gap between the solid wall and the computational domain for the fluid and temperature fields. See Wall Boundary Conditions described for The Algebraic yPlus Turbulence Model and The k-ε Turbulence Model). This theoretical gap applies also to the temperature fields but is most often ignored when the computational geometry is drawn.

Standard The standard temperature wall function takes into account conduction in the boundary layer. The heat flux between the fluid with temperature T_f and a wall with temperature T_w, is

$$q_{wf} = \frac{\rho C_p u_\tau (T_w - T_f)}{T^+}$$

where ρ is the fluid density, C_p is the fluid heat capacity, and u_τ is the friction velocity. T^+ is the dimensionless temperature and is given by (Ref. 6)

$$T^+ = \begin{cases} \mathrm{Pr}\delta_w^+ & \text{for } \delta_w^+ < \delta_{w1}^+ \\ 15\mathrm{Pr}^{2/3} - \dfrac{500}{\delta_w^{+2}} & \text{for } \delta_{w1}^+ \le \delta_w^+ < \delta_{w2}^+ \\ \dfrac{\mathrm{Pr}_T}{\kappa}\ln\delta_w^+ + \beta & \text{for } \delta_{w2}^+ \le \delta_w^+ \end{cases}$$

where, in turn,

$$\delta_w^+ = \frac{\delta_w \rho \sqrt{C_\mu^{1/2} k}}{\mu} \qquad \delta_{w1}^+ = \frac{10}{\mathrm{Pr}^{1/3}}$$

$$\delta_{w2}^+ = 10\sqrt{10\frac{\kappa}{\mathrm{Pr}_T}} \qquad \mathrm{Pr} = \frac{C_p\mu}{\lambda}$$

$$\beta = 15\mathrm{Pr}^{2/3} - \frac{\mathrm{Pr}_T}{2\kappa}\left(1 + \ln\left(1000\frac{\kappa}{\mathrm{Pr}_T}\right)\right)$$

λ is the thermal conductivity, and κ is the von Kármán constant equal to 0.41.

High viscous dissipation at wall Launder and Spalding propose a temperature wall function that accounts for conduction as well as viscous dissipation. The heat flux is written

$$q_{wf} = \begin{cases} \dfrac{\rho u_\tau}{\mathrm{Pr}u^+}\left[C_p(T_w - T_f) - \dfrac{1}{2}\mathrm{Pr}U^2\right] & \text{for } \delta_w^+ < \delta_{wc}^+ \\ \dfrac{\rho u_\tau}{\mathrm{Pr}_T(u^+ + P)}\left[C_p(T_w - T_f) - \dfrac{1}{2}(\mathrm{Pr}U_c^2 + \mathrm{Pr}_T(U^2 - U_c^2))\right] & \text{for } \delta_w^+ \ge \delta_{wc}^+ \end{cases}$$

Variables with an index "c" are evaluated at the critical distance, which corresponds to the switch from the laminar sublayer to the logarithmic layer. The critical wall distance $\delta_w{}^+_c$, which depends on the turbulent parameters κ and B, is estimated from a second-order accurate solution:

$$\delta_{wc}^+ = \frac{X_0}{\kappa}\left[2 - X_0 + \sqrt{(X_0 - 1)^2 + 2\left(-\kappa_0 B_0 + \kappa B - \ln\left(\frac{\kappa}{\kappa_0}\right)\right)}\right]$$

with $\kappa_0 = 0.41$, $B_0 = 5.2$, and $X_0 = 4.53554291157957$.

The velocity at $\delta_w{}^+_c$ is then calculated from a velocity wall function, according to the turbulence model and wall treatment chosen to keep consistency. The velocity wall

function used for the determination of U_c when the L-VEL or a LES turbulence model is chosen is based on a blending of the linear and logarithmic laws. It gives very similar results to the wall function actually used for the calculation of the velocity at the first cell which is based on the wall Reynolds number.

P is a measure of the resistance of the boundary layer to heat transport, and is estimated with Jayatilleke's formula:

$$P = 9.21\left[\left(\frac{\mathrm{Pr}}{\mathrm{Pr}_T}\right)^{3/4} - 1\right]\left[1 + 0.28\exp\left(-0.007\frac{\mathrm{Pr}}{\mathrm{Pr}_T}\right)\right]$$

The distance between the computational fluid domain and the wall, δ_w, is always $h_w/2$ for automatic wall treatment where h_w is the height of the mesh cell adjacent to the wall. $h_w/2$ is almost always very small compared to any geometrical quantity of interest, at least if a boundary layer mesh is used. For wall function, δ_w is at least $h_w/2$ and can be bigger if necessary to keep δ_w^+ higher than 11.06. The computational results should be checked so that the distance between the computational fluid domain and the wall, δ_w, is everywhere small compared to any geometrical quantity of interest. The distance δ_w is available for evaluation on boundaries.

The Boussinesq Approximation

The Boussinesq approximation assumes that density variations only contribute to buoyancy effects, of which thermal effects are considered herein

$$\rho = \rho_0(1 - \alpha_p(T_0)(T - T_0)) \tag{4-17}$$

where ρ_0, α, and T_0 are constants and T is the temperature. Constant temperature and pressure are assumed when evaluating all other material properties. Provided that α_p and $T - T_0$ are small enough, Equation 4-1 and Equation 4-2 reduce to

$$\begin{gathered}\rho_0\nabla\cdot\mathbf{u} = 0\\ \rho_0\frac{\partial\mathbf{u}}{\partial t} + \rho_0\mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \mu_0\nabla\cdot(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \mathbf{F}\\ \rho_0 C_{p0}\left(\frac{\partial T}{\partial t} + (\mathbf{u}\cdot\nabla)T\right) = (\nabla\cdot K_0\nabla T) + \tau{:}\mathbf{S} + Q\end{gathered} \tag{4-18}$$

where K_0 is the constant thermal conductivity.

The Boussinesq approximation is commonly used to simulate buoyancy-driven flows. In this case

$$\mathbf{F} = (\rho_0 + \Delta\rho)\mathbf{g} = -\rho_0(1-\alpha_p(T_0)(T-T_0))\mathbf{g} \quad (4\text{-}19)$$

where $\mathbf{g}$ is the gravity vector. A further useful simplification is possible by writing Equation 4-19 in terms of a potential, Φ:

$$\mathbf{F} = -\nabla(\rho_0\Phi) + \Delta\rho\mathbf{g}$$

The first part can be canceled out by splitting the true pressure, p, into a hydrodynamic component, P, and a hydrostatic component, $-\rho_0\Phi$ such that $P = p + \rho_0\Phi$. This reduced Equation 4-18 to

$$\begin{gathered}\rho_0\nabla\cdot\mathbf{u} = 0\\ \rho_0\frac{\partial\mathbf{u}}{\partial t} + \rho_0\mathbf{u}\cdot\nabla\mathbf{u} = -\nabla P + \mu_0\nabla\cdot(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho_0\alpha_p(T_0)(T-T_0)\mathbf{g} \quad (4\text{-}20)\\ \rho_0 C_{p0}\left(\frac{\partial T}{\partial t} + (\mathbf{u}\cdot\nabla)T\right) = (\nabla\cdot K_0\nabla T) + \tau{:}\mathbf{S} + Q\end{gathered}$$

The gravity force is added on the form given by Equation 4-19 if **Include gravity** is selected in the fluid flow interface. The form in Equation 4-20 is obtained when selecting the **Use reduced pressure** option.

When an LES turbulence model is applied, an additional contribution,

$$\rho_0\alpha_p(T_0)T'\mathbf{g}$$

is added to the buoyancy force in Equation 4-19 and Equation 4-20.

The main assumption in the Boussinesq approximation is that the density fluctuations must be small; that is, $\Delta\rho/\rho_0 << 1$. There are also some more subtle constraints that, for example, make the Boussinesq approximation unsuitable for systems of very large dimensions. It can also be observed the energy equation in Equation 4-20 retains both the viscous heating term and the pressure work term. These can, however, almost always be neglected in situations when the Boussinesq approximation is valid (see, for example, Ref. 7). But there are situations where they need to be retained (Ref. 8). In particular, the pressure work term can be of importance for liquids where $C_p \neq C_v$ (Ref. 9). An excellent discussion of the Boussinesq approximation and its limitations appears in Chapter 14 of Ref. 7.

Theory for the Nonisothermal Screen Boundary Condition

When the Nonisothermal Flow multiphysics coupling feature is active, the conditions that apply across a screen in isothermal flow are complemented by

$$[H_0]^+_- = 0 \tag{4-21}$$

where H_0 is the total enthalpy.

- See Screen for the feature node details.
- Also see Screen Boundary Condition described for the single-phase flow interfaces.

Theory for the Interior Fan Boundary Condition

When the Nonisothermal Flow multiphysics coupling feature is active, the temperature field is discontinuous over the fan and the conditions that apply across an interior fan are complemented by:

- If direction is Along normal vector, the outlet temperature T_{avg} is defined by

$$\left(\int_\Gamma \text{up}(\mathbf{u}\cdot\mathbf{n}\rho C_p)dS\right)T_{\text{avg}} = \int_\Gamma \text{down}(\mathbf{u}\cdot\mathbf{n}\rho C_p T)dS$$

- If the direction is opposite to normal vector, the outlet temperature T_{avg} is defined by

$$\left(\int_\Gamma \text{down}(\mathbf{u}\cdot\mathbf{n}\rho C_p)dS\right)T_{\text{avg}} = \int_\Gamma \text{up}(\mathbf{u}\cdot\mathbf{n}\rho C_p T)dS$$

References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

1. D.C. Wilcox, *Turbulence Modeling for CFD*, 2nd ed., DCW Industries, 1998.

2. J. Larsson, *Numerical Simulation of Turbulent Flows for Turbine Blade Heat Transfer*, Doctoral Thesis for the Degree of Doctor of Philosophy, Chalmers University of Technology, Sweden, 1998.

3. R.L. Panton, *Incompressible Flow*, 2nd ed., John Wiley & Sons, 1996.

4. W.M. Kays, "Turbulent Prandtl Number — Where Are We?", *ASME Journal of Heat Transfer*, vol. 116, pp. 284–295, 1994.

5. B. Weigand, J.R. Ferguson, and M.E. Crawford, "An Extended Kays and Crawford Turbulent Prandtl Number Model," *Int. J. Heat and Mass Transfer*, vol. 40, no. 17, pp. 4191–4196, 1997.

6. D. Lacasse, È. Turgeon, and D. Pelletier, "On the Judicious Use of the k-ε Model, Wall Functions and Adaptivity," *Int. J. Thermal Sciences,* vol. 43, pp. 925–938, 2004.

7. D.J. Tritton, *Physical Fluid Dynamics*, 2nd ed., Clarendon Press, 1988.

8. D.D. Gray and A. Giorgini, "The Validity of the Boussinesq Approximation for Liquids and Gases," *Int. J. Heat and Mass Transfer*, vol. 19, pp. 545–551, 1967.

9. P.G. Drazin and W.H. Reid, *Hydrodynamic stability*, Cambridge University Press, 1981.

Theory for the Nonisothermal Viscoelastic Flow

The theory for the Viscoelastic Flow interface is described in this section:

- Nonisothermal Viscoelastic Flow Theory
- References for the Nonisothermal Viscoelastic Flow Interfaces

Nonisothermal Viscoelastic Flow Theory

In many industrial application involving the polymer processing, the flow conditions are nonisothermal. The material properties of viscoelastic fluids, such as viscosity and relaxation time show significant temperature dependence. Therefore, the viscoelastic stress depends on the temperature distribution. Another important aspect to consider is the internal heat production.

The **Nonisothermal Flow, Viscoelastic Flow** interface contains the equation for the flow of viscoelastic fluid:

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{4-22}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} \tag{4-23}$$

where

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is the pressure (SI unit: Pa)
- $\mathbf{F}$ is the body force vector (SI unit: N/m^3)
- τ is the extra stress tensor (SI unit: Pa).

The extra stress tensor is defined as a sum of a viscous and a viscoelastic contribution as

$$\tau = 2\mu_s \mathbf{S} + \mathbf{T}_e \tag{4-24}$$

where μ_s is the solvent viscosity, $\mathbf{S}$ is the strain-rate tensor, and $\mathbf{T}_e$ is the elastic stress tensor that can be represented as a sum of the individual modes. The system of

equations Equation 4-22-Equation 4-23 needs to be supplemented by the constitutive model for the viscoelastic stress.

Nonisothermal Flow, Viscoelastic Flow also adds the heat equation which for a viscoelastic fluid is given by

$$\rho C_p\left(\frac{\partial T}{\partial t} + (\mathbf{u}\cdot\nabla)T\right) = -(\nabla\cdot\mathbf{q}) + \tau:\mathbf{S} + Q \tag{4-25}$$

where

- C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- $\mathbf{q}$ is the heat flux by conduction (SI unit: W/m^2)
- τ is the extra stress tensor (SI unit: Pa) given by (Equation 4-24)
- $\mathbf{S}$ is the strain-rate tensor (SI unit: 1/s)
- Q contains heat sources other than viscous heating (SI unit: W/m^3)

Generally speaking, for viscoelastic flows, the internal heat production term consists of an irreversible dissipation part and a reversible part (Ref. 1). The reversible part of the internal heat production is neglected in the Equation 4-2. The irreversible part is given by

$$\tau:\mathbf{S} \tag{4-26}$$

For inelastic constitutive models, the irreversible losses are equal to the viscous dissipation.

References for the Nonisothermal Viscoelastic Flow Interfaces

1. G.W.M. Peters and F.P.T. Baaijens, "Modelling of non-isothermal viscoelastic flows," *J. Nonnewton. Fluid. Mech.*, vol. 68, pp. 205–224, 1997.

5

High Mach Number Flow Interfaces

This chapter discusses physics interfaces found under the **Fluid Flow** > **High Mach Number Flow** branch ( ).

In this chapter:

- The High Mach Number Flow Interfaces
- The Compressible Euler Equations Interface
- The Rotating Machinery, High Mach Number Flow Interfaces
- Theory for the High Mach Number Flow Interfaces
- Theory for the Compressible Euler Equations Interface

The High Mach Number Flow Interfaces

There are twelve versions of the same predefined multiphysics interface (all with the name `hmnf`) that combine the heat equation with either the laminar or turbulent flow equations. The advantage of using the multiphysics interfaces — compared to adding the individual physics interfaces separately — is that a set of two-way couplings has been predefined. Solving this coupled system of equations usually requires numerical stabilization, which the predefined multiphysics interface also sets up.

These physics interfaces vary only by one or two default settings (see Table 5-1) or selections from checkboxes or lists under the **Physical Model** and **Turbulence** sections for the physics interface.

TABLE 5-1: THE HIGH MACH NUMBER FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	TURBULENCE MODEL TYPE	TURBULENCE MODEL	HEAT TRANSPORT TURBULENCE MODEL
High Mach Number Flow, Laminar	hmnf	None	N/A	N/A
High Mach Number Flow, Algebraic yPlus	hmnf	RANS-EVM	Algebraic yPlus	Kays–Crawford
High Mach Number Flow, L-VEL	hmnf	RANS-EVM	L-VEL	Kays–Crawford
High Mach Number Flow, k-ε	hmnf	RANS-EVM	k-ε	Kays–Crawford
High Mach Number Flow, Realizable k-ε	hmnf	RANS-EVM	Realizable k-ε	Kays–Crawford
High Mach Number Flow, k-ω	hmnf	RANS-EVM	k-ω	Kays–Crawford
High Mach Number Flow, SST	hmnf	RANS-EVM	SST	Kays–Crawford
High Mach Number Flow, Low Reynolds Number k-ε	hmnf	RANS-EVM	Low Reynolds number k-ε	Kays–Crawford
High Mach Number Flow, Spalart–Allmaras	hmnf	RANS-EVM	Spalart–Allmaras	Kays–Crawford

TABLE 5-1: THE HIGH MACH NUMBER FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	TURBULENCE MODEL TYPE	TURBULENCE MODEL	HEAT TRANSPORT TURBULENCE MODEL
High Mach Number Flow, v2-f	hmnf	RANS-EVM	v2-f	Kays–Crawford
High Mach Number Flow, Wilcox R-ω	hmnf	RANS-RSM	Wilcox R-ω	Kays–Crawford
High Mach Number Flow, SSG-LRR	hmnf	RANS-RSM	SSG-LRR	Kays–Crawford

Most of the other physics nodes share the same setting options as described in this section and in Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces. See also The Heat Transfer in Solids Interface in the *Heat Transfer Module User's Guide* for details about the Heat Transfer in Solids physics node.

- The High Mach Number Flow, Laminar Interface
- The High Mach Number Flow, k-ε Interface
- The High Mach Number Flow, Spalart–Allmaras Interface
- The High Mach Number Flow, Algebraic yPlus Interface
- The High Mach Number Flow, L-VEL Interface
- The High Mach Number Flow, Realizable k-ε Interface
- The High Mach Number Flow, k-ω Interface
- The High Mach Number Flow, SST Interface
- The High Mach Number Flow, Low Reynolds Number k-ε Interface
- The High Mach Number Flow, v2-f Interface
- The High Mach Number Flow, Wilcox R-ω Interface
- The High Mach Number Flow, SSG-LRR Interface
- Theory for the High Mach Number Flow Interfaces

The High Mach Number Flow, Laminar Interface

The **High Mach Number Flow, Laminar (hmnf)** interface (), found under the **Fluid Flow** > **High Mach Number Flow** branch () when adding a physics interface, is used to model gas flows at low and moderate Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, laminar flows in the transonic and supersonic range. This state is often connected to very low pressures.

The physics interface solves for conservation of energy, mass, and momentum. The interface also supports heat transfer in solids as well as surface-to-surface radiation.

This physics interface is a predefined multiphysics coupling consisting of a Laminar Flow interface, applied to compressible flow, in combination with a Heat Transfer interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall, Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `hmnf`.

PHYSICAL MODEL

The **Reference temperature** T_{ref} is used to define the reference enthalpy H_{ref} which is set to 0 J/kg at T_{ref}. When the **Include kinetic energy** checkbox is selected, the conservative total-energy equation is solved.

TURBULENCE

Turbulence Model Type

By definition, no turbulence model is needed when studying laminar flows. The default is **None**. Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM** or **RANS-RSM**.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). The names can be changed but the names of fields and dependent variables must be unique within a component.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** checkbox to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** calculates the local CFL number (from the Courant–Friedrichs–Lewy condition) from a built-in expression. For **Manual** enter a **Local CFL number** $\mathrm{CFL}_{\mathrm{loc}}$.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
- The Heat Transfer Module Interfaces
- The High Mach Number Flow, k-ε Interface

The High Mach Number Flow, k-ε Interface

The **High Mach Number Flow, k-ε (hmnf)** interface ( ), found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface, is used to model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow and heat transfer close to walls are modeled using wall

functions. The physics interface also supports heat transfer in solids as well as surface-to-surface radiation.

This is a predefined multiphysics interface combining k-ε turbulence model for compressible flow with a heat transfer model. As shown in Table 5-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default turbulence model selected — **k-ε** for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall**, **Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `hmnf`.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**, the default **Turbulence model** is **k-ε**, and the default **Heat transport turbulence model** is **Kays–Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

Edit Turbulence Model Parameters

Edit the model parameters of the k-ε model as needed. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling and heat radiation, the **Turbulent kinetic energy** k (SI unit: m^2/s^2) and **Turbulent dissipation rate** ep (SI unit: m^2/s^3) variables are also available.

The names can be changed but the names of fields and dependent variables must be unique within a model.

- The Heat Transfer Module Interfaces in the *Heat Transfer Module User's Guide*
- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
- The High Mach Number Flow, Laminar Interface

The High Mach Number Flow, Spalart–Allmaras Interface

The **High Mach Number Flow, Spalart–Allmaras (hmnf)** interface (), found under the **High Mach Number Flow** > **Turbulent Flow** branch () when adding a physics interface, is used to model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the one-equation Spalart–Allmaras turbulence model. The Spalart–Allmaras model is a so-called low-Reynolds number model, which means that it resolves the velocity, pressure, and temperature fields all the way down to the wall. The Spalart–Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation. It also supports heat transfer in solids as well as surface-to-surface radiation.

This is a predefined multiphysics interface which combines a turbulence Spalart–Allmaras model for compressible flow with a heat transfer model. As shown in Table 5-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default Turbulence model selected — **Spalart–Allmaras** for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall**, **Thermal Insulation**, and **Initial Values**. Then, from the

Physics toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**, the default **Turbulence model** is **Spalart–Allmaras**, and the default **Heat transport turbulence model** is **Kays–Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling and heat radiation, the **Reciprocal wall distance** G (SI unit: 1/m) and **Undamped turbulent kinematic viscosity** nutilde (SI unit: m^2/s) variables are also available.

- The Heat Transfer Module Interfaces in the *Heat Transfer Module User's Guide*
- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
- The High Mach Number Flow, Laminar Interface

Transonic Flow in a Sajben Diffuser: Application Library path **CFD_Module/High_Mach_Number_Flow/sajben_diffuser**

The High Mach Number Flow, Algebraic yPlus Interface

The **High Number Flow, Algebraic yPlus (hmnf)** interface ( ) is found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface. This is a predefined multiphysics interface which combines The Turbulent Flow, Algebraic yPlus Interface for compressible flow with The Heat Transfer Module Interfaces.

A detailed description of the **High Number Flow, Algebraic yPlus (hmnf)** interface, which models turbulent gas flows in the transonic and supersonic range, is analogous to The High Mach Number Flow, k-ε Interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow, L-VEL Interface

The **High Number Flow, L-VEL (hmnf)** interface ( ) is found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface. This is a predefined multiphysics interface which combines The Turbulent Flow, L-VEL Interface for compressible flow with The Heat Transfer Module Interfaces.

A detailed description of the **High Number Flow, L-VEL (hmnf)** interface, which models turbulent gas flows in the transonic and supersonic range, is analogous to The High Mach Number Flow, k-ε Interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow, Realizable k-ε Interface

The **High Number Flow, Realizable k-ε (hmnf)** interface ( ) is found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface. This is a predefined multiphysics interface which combines The Turbulent Flow, Realizable k-ε Interface for compressible flow with The Heat Transfer Module Interfaces.

A detailed description of the **High Number Flow, Realizable k-ε (hmnf)** interface, which models turbulent gas flows in the transonic and supersonic range, is analogous to The High Mach Number Flow, k-ε Interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow, k-ω Interface

The **High Number Flow, k-ω (hmnf)** interface ( ) is found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface. This is a predefined multiphysics interface which combines The Turbulent Flow, k-ω Interface for compressible flow with The Heat Transfer Module Interfaces.

A detailed description of the **High Number Flow, k-ω (hmnf)** interface, which models turbulent gas flows in the transonic and supersonic range, is analogous to The High Mach Number Flow, k-ε Interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow, SST Interface

The **High Number Flow, SST (hmnf)** interface ( ) is found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface. This is a predefined multiphysics interface which combines The Turbulent Flow, SST Interface for compressible flow with The Heat Transfer Module Interfaces.

A detailed description of the **High Number Flow, SST (hmnf)** interface, which models turbulent gas flows in the transonic and supersonic range, is analogous to The High Mach Number Flow, k-ε Interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow, Low Reynolds Number k-ε Interface

The **High Number Flow, Low Reynolds Number k-ε (hmnf)** interface ( ) is found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface. This is a predefined multiphysics interface which combines The Turbulent Flow, Low Re k-ε Interface for compressible flow with The Heat Transfer Module Interfaces.

A detailed description of the **High Number Flow, Low Reynolds Number k-ε (hmnf)** interface, which models turbulent gas flows in the transonic and supersonic range, is analogous to The High Mach Number Flow, k-ε Interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow, v2-f Interface

The **High Number Flow, v2-f (hmnf)** interface ( ) is found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface. This is a predefined multiphysics interface which combines The Turbulent Flow, v2-f Interface for compressible flow with The Heat Transfer Module Interfaces.

A detailed description of the **High Number Flow, v2-f (hmnf)** interface, which models turbulent gas flows in the transonic and supersonic range, is analogous to The High Mach Number Flow, k-ε Interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow, Wilcox R-ω Interface

The **High Mach Number Flow, Wilcox R-ω (hmnf)** interface ( ), found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface, is used to model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the Wilcox R-ω model, which solves six transport equations for the turbulence Reynolds stress tensor and a transport equation for the specific dissipation rate. Flow and heat transfer close to walls are modeled using **Low Re** wall treatment, which enforces resolution all the way down to the wall and, hence, demands quite fine mesh near the wall. The physics interface also supports heat transfer in solids as well as surface-to-surface radiation.

This is a predefined multiphysics interface combining Wilcox R-ω turbulence model for compressible flow with a heat transfer model. As shown in Table 5-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default turbulence model selected — **Wilcox R-ω** for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall**, **Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

TURBULENCE

The default **Turbulence model type** is **RANS-RSM**, the default **Turbulence model** is **Wilcox R-ω**, and the default **Heat transport turbulence model** is **Kays–Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

Edit Turbulence Model Parameters

Edit the model parameters of the **Wilcox R-ω** model as needed. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling and heat radiation, the six components of **Kinematic Reynolds stress** uu, vv, ww, uv, uw, vw (SI unit: m^2/s^2), the **Specific dissipation rate** om (SI unit: 1/s), and the **Reciprocal wall distance** G (SI unit: 1/m) variables are also available.

The names can be changed but the names of fields and dependent variables must be unique within a model.

- The Heat Transfer Module Interfaces in the *Heat Transfer Module User's Guide*
- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
- The High Mach Number Flow, Laminar Interface

The High Mach Number Flow, SSG-LRR Interface

The **High Mach Number Flow, SSG-LRR (hmnf)** interface ( ), found under the **High Mach Number Flow** > **Turbulent Flow** branch ( ) when adding a physics interface, is used to model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the Speziale-Sarkar-Gatski/Launder-Reece-Rodi-ω (SSG-LRR) model, which solves six transport equations for the turbulence Reynolds stress tensor and a transport equation for the specific dissipation rate. Flow and heat transfer close to walls are modeled using **Low Re** wall treatment, which enforces resolution all the way down to the wall and, hence, demands quite fine mesh near the wall. The physics interface also supports heat transfer in solids as well as surface-to-surface radiation.

This is a predefined multiphysics interface combining SSG-LRR turbulence model for compressible flow with a heat transfer model. As shown in Table 5-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default turbulence model selected — **SSG-LRR** for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall**, **Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

TURBULENCE

The default **Turbulence model type** is **RANS-RSM**, the default **Turbulence model** is **SSG-LRR**, and the default **Heat transport turbulence model** is **Kays–Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

Edit Turbulence Model Parameters

Edit the model parameters of the **SSG-LRR** model as needed. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling and heat radiation, the six components of **Kinematic Reynolds stress** uu, vv, ww, uv, uw, vw (SI unit: m^2/s^2), and the **Specific dissipation rate** om (SI unit: 1/s), and the **Reciprocal wall distance** G (SI unit: 1/m) variables are also available.

The names can be changed but the names of fields and dependent variables must be unique within a model.

- The Heat Transfer Module Interfaces in the *Heat Transfer Module User's Guide*
- Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
- The High Mach Number Flow, Laminar Interface

Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow Interfaces has these domain, boundary, edge, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics**

context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

The following nodes are slightly different from those in the other physics interfaces and are described in this section (listed in alphabetical order):

- Continuity
- Fluid
- Initial Values
- Inlet
- Outlet
- Periodic Condition
- Symmetry
- Generate New Turbulence Model Interface

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface:

- Volume Force
- Wall
- Interior Wall
- Pressure Point Constraint

The Interior Wall feature requires appropriate conditions for the temperature. Use a Thermal Insulation or Temperature node together with Interior Wall to get appropriate boundary conditions for all the flow and heat variables.

For The High Mach Number Flow, k-ε Interface, the same nodes are selected from the **Turbulent Flow, k-ε** submenus. For The High Mach Number Flow, Spalart–Allmaras Interface, the same nodes are selected from the **Turbulent Flow, Spalart–Allmaras** submenus.

The following physics nodes and subnodes (listed in alphabetical order) are described for the Heat Transfer interfaces in the *Heat Transfer Module User's Guide*. Additional features can also be available when you have additional licenses:

- Boundary Heat Source
- Heat Flux
- Heat Source
- Solid
- Line Heat Source
- Periodic Condition (Heat Transfer Interface)
- Point Heat Source
- Diffuse Surface (Surface-to-Surface Radiation Interface)
- Temperature
- Thermal Insulation
- Thin Layer (Heat Transfer Interface) and Solid (Heat Transfer in Shells Interface)

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Continuity

The **Continuity** node can be added to pair boundaries. It prescribes that the flow and temperature fields are continuous across the boundary. Flow characteristics at the boundary, described in Plane Wave Analysis of Inviscid Flow, are utilized to implement the continuity of the flow and temperature fields. When added to pair boundaries, the **Continuity** feature is applicable where the boundaries match, that is, when the source boundary has a corresponding destination boundary and vice-versa. Elsewhere in the pair boundaries, the **Fallback** feature is activated.

About Pairs

PAIR SELECTION

If this node is selected from the **Pairs** menu, choose the pair to apply this condition to. A pair must be created first. See Identity, Contact, and Sector Symmetry Pairs in the *COMSOL Multiphysics Reference Manual* for more details.

Initial Values

The **Initial Values** node adds initial values for the velocity field, the pressure and the temperature that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver. For turbulent flow there are also initial values for the turbulence model variables. The surface radiosity is only applicable for surface-to-surface radiation.

INITIAL VALUES

Enter values or expressions for the initial value of the **Velocity field** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). The default values are 0 m/s for the velocity, 1 atm for the pressure, and 293.15 K for the temperature.

In a turbulent flow interface, initial values for the turbulence variables are also specified. By default these are specified using the predefined variables defined by the expressions described in Theory for the High Mach Number Flow Interfaces under Initial Values.

Fluid

The **Fluid** node adds the continuity, momentum, and temperature equations for an ideal gas but omits volume forces and heat sources. Volume forces and heat sources can be added as separate physics features. Viscous heating and pressure work terms are added by default to the temperature equation.

When the turbulence model type is set to **RANS-EVM** or **RANS-RSM**, the Fluid node also adds the equations for the turbulence variables.

HEAT CONDUCTION

Fourier's law of heat conduction gives the relation between the heat flux vector $\mathbf{q}$ and the temperature gradient ∇T, as $\mathbf{q} = -k\nabla T$. Select a **Thermal conductivity** k (SI unit: W/(m·K)) from the list — **Sutherland's Law** (the default), **From material**, or **User defined**. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the thermal conductivity and enter another value or expression in the field or matrix.

Sutherland's Law

For **Sutherland's Law** enter the following model parameters:

- **Conductivity at reference temperature** k_{ref} (SI unit: W/(m·K))
- **Reference temperature** $T_{\mathrm{k,ref}}$ (SI unit: K)

- **Sutherland constant** S_k (SI unit: K)

Sutherland's law describes the relationship between the thermal conductivity and the total temperature of an ideal fluid according to

$$k = k_{\text{ref}}\left(\frac{T}{T_{k,\text{ref}}}\right)^{3/2}\frac{T_{k,\text{ref}}+S_k}{T+S_k}$$

THERMODYNAMICS

The High Mach Number Flow interface is applicable for ideal gases. Specify the thermodynamics properties by selecting a gas constant type and selecting between entering the heat capacity at constant pressure or the ratio of specific heats. For an ideal gas the density is defined as

$$\rho = \frac{M_n p_A}{RT} = \frac{p_A}{R_s T}$$

where p_A is the absolute pressure, and T is the temperature.

- Select a **Gas constant type** — **Specific gas constant** R_s (SI unit: J/(kg·K)) or **Mean molar mass** M_n (SI unit: kg/mol). The default setting is to use the property value **From material**. For **User defined** enter another value or expression for either material property. For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K), which is a built-in physical constant, is also used.
- From the **Specify Cp or** γ list, select **Heat capacity at constant pressure** C_p (SI unit: J/(kg·K)) or **Ratio of specific heats** γ (dimensionless). The default setting is to use the property value **From material**. For **User defined** enter another value or expression for either material property.

DYNAMIC VISCOSITY

The dynamic viscosity describes the relationship between the shear rate and the shear stresses in a fluid.

Select a **Dynamic viscosity** μ (SI unit: Pa·s) from the list — **Sutherland's Law** (the default), **From material**, or **User defined**.

Sutherland's Law

For **Sutherland's Law** enter the following model parameters:

- **Dynamic viscosity at reference temperature** μ_{ref} (SI unit: Pa·s)

- **Reference temperature** $T_{\mu,\mathrm{ref}}$ (SI unit: K)
- **Sutherland constant** S_μ (SI unit: K)

Sutherland's law describes the relationship between the dynamic viscosity and the total temperature of an ideal fluid according to

$$\mu = \mu_{\mathrm{ref}}\left(\frac{T}{T_{\mu,\,\mathrm{ref}}}\right)^{3/2}\frac{T_{\mu,\,\mathrm{ref}}+S_\mu}{T+S_\mu}$$

MIXING LENGTH LIMIT

This section is available for turbulence models using **Wall functions** for **Wall treatment**.

These turbulence models need an upper limit on the mixing length to be numerically robust. Select a **Mixing length limit** — **Automatic** (the default) or **Manual**.

- For **Automatic** this limit is automatically evaluated as:

$$l_{\mathrm{mix}}^{\mathrm{lim}} = 0.5 l_{bb} \tag{5-1}$$

  where l_{bb} is the shortest side of the geometry bounding box. If the geometry is a complicated system of very slender entities, for example, Equation 5-1 tends to give a result that is too large. In such cases, define $l_{\mathrm{mix}}^{\mathrm{lim}}$ manually.
- For **Manual** enter a value or expression for the **Mixing length limit** $l_{\mathrm{mix}}^{\mathrm{lim}}$ (SI unit: m).

DISTANCE EQUATION

This section is available for turbulence models including a Wall Distance interface.

Select how the **Reference length scale** l_{ref} (SI unit: m) is defined — **Automatic** (default) or **Manual**:

- For **Automatic** the wall distance is automatically evaluated to one tenth of the shortest side of the geometry bounding box. This is usually quite accurate but it can sometimes give a too high value if the geometry consists of several slim entities. In such cases, define the reference length scale manually.
- For **Manual** it defines a different value or expression for the length scale. The default is 1 m.

l_{ref} controls the result of the distance equation. Objects that are much smaller than l_{ref} are effectively be diminished while the distance to objects much larger than l_{ref} are accurately represented.

Inlet

The **Inlet** node includes a set of boundary conditions describing the fluid flow and temperature conditions at an inlet. The applied conditions are controlled by the **Flow Condition**.

FLOW CONDITION

Select a **Flow condition** — **Characteristics based** (the default), **Supersonic** or **Subsonic**.

For **Characteristics based** the current flow situation is analyzed using the inviscid flow characteristics at the inlet. This can be used to specify either a subsonic ($\mathrm{Ma} < 1$) inlet or a supersonic inlet ($\mathrm{Ma} > 1$).

FLOW PROPERTIES

When the **Flow condition** is set to **Characteristics based** or **Supersonic**, specify the flow properties at the inlet in terms of the static or total pressure, static or total temperature, Mach number, and flow direction. By default **Static** input variables are used.

Select an **Input state** — **Static** (the default) or **Total**. For either selection also enter values or expressions for the **Mach number** Ma_0 (dimensionless) at the inlet. The default is 1.5.

- For **Static** enter values or expressions for the **Static pressure** $p_{0,\mathrm{stat}}$ (SI unit: Pa) and **Static temperature** $T_{0,\mathrm{stat}}$ (SI unit: K).
- For **Total** enter values or expressions for the **Total pressure** $p_{0,\mathrm{tot}}$ (SI unit: Pa) and **Total temperature** $T_{0,\mathrm{tot}}$ (SI unit: K).

The relationships between the static and total states are:

$$\begin{aligned} \frac{p_{\mathrm{tot}}}{p_{\mathrm{stat}}} &= \left(1 + \frac{\gamma - 1}{2}\mathrm{Ma}^2\right)^{\frac{\gamma}{\gamma - 1}} \\ \frac{T_{\mathrm{tot}}}{T_{\mathrm{stat}}} &= \left(1 + \frac{\gamma - 1}{2}\mathrm{Ma}^2\right) \end{aligned} \tag{5-2}$$

Select a **Flow direction** — **Normal inflow** (the default) or **User defined** to specify an arbitrary flow direction. Then enter the components of the direction normal n_{M} (dimensionless).

When the **Flow condition** is set to **Subsonic**, choose to specify either **Velocity** or **Pressure**. For **Velocity**, enter a value or expression for U_0 (SI unit: m / s). For **Pressure**, enter a value or expression for p_0 (SI unit: Pa). The **Suppress backflow** option is enabled by

default. Select a **Flow direction** — **Normal inflow** (the default) or **User defined**. Choose to specify either **Temperature** or **Heat flux**. For **Temperature**, enter a value or expression for T_0 (SI unit: K). For **Heat flux**, enter a value or expression for T_{ustr} (SI unit: K).

TURBULENCE PROPERTIES

This section displays when **RANS-EVM** or **RANS-RSM** is selected as **Turbulence model type**.

Turbulence properties at an inlet can be specified according to one of the following options:

- Select **Specify turbulence length scale and intensity** to enter values or expressions for the **Turbulent intensity** I_T (dimensionless) and **Turbulence length scale** L_T (SI unit: m). I_T and L_T values are related to the turbulence variables via

$$k = \frac{3}{2}(|\mathbf{U}|I_T)^2, \qquad \varepsilon = C_\mu^{3/4}\frac{k^{3/2}}{L_T}$$

- For **Specify turbulence variables** enter values or expressions for the turbulence variables, such as **Turbulent kinetic energy** k_0 (SI unit: m^2/s^2), **Turbulent dissipation rate**, ε_0 (SI unit: m^2/s^3), **Specific dissipation rate**, ω_0 (SI unit: $1/s$), **Kinematic Reynolds stress tensor** R_0 (SI unit: m^2/s^2), **Undamped turbulent kinematic viscosity**, v_0 (SI unit: m^2/s), **Turbulent relative fluctuations**, ζ_0 (dimensionless), **Elliptic blending function**, α_0 (dimensionless) and **Intermittency**, γ_0 (dimensionless) depending on the choice of **Turbulence model**.

For background on the derivation and implementation of the conditions, see Theory for the High Mach Number Flow Interfaces.

For recommendations of physically sound values see Inlet Values for the Turbulence Length Scale and Turbulent Intensity.

Outlet

The **Outlet** node includes a set of boundary conditions describing fluid flow and temperature conditions at an outlet. The applied conditions are controlled by the **Flow Condition**.

FLOW CONDITION

Select a **Flow condition** — **Hybrid** (the default), **Supersonic**, or **Subsonic**.

- Using a **Hybrid** condition, both subsonic ($\mathrm{Ma} < 1$) and supersonic flow ($\mathrm{Ma} > 1$) conditions at the outlet are supported.
- Select **Supersonic** when the flow at the outlet is known to be supersonic.
- Select **Subsonic** when the flow at the outlet is known to be subsonic.

FLOW PROPERTIES

This section displays when the **Hybrid** or **Subsonic** flow condition is selected.

Hybrid

For **Hybrid** an outlet pressure is specified. This pressure is enforced at the outlet when the flow is subsonic. Select an **Input state** — **Static** (the default) or **Total**. The relation between the static and total pressure is defined in Equation 5-2.

- For **Static** enter a value or expression for the **Static pressure** $p_{0,\mathrm{stat}}$ (SI unit: Pa). The default is 1 atm.
- For **Total** enter a value or expression for the **Total pressure** $p_{0,\mathrm{tot}}$ (SI unit: Pa). The default is 1 atm.

Subsonic

For **Subsonic** select the **Boundary condition** — **Normal Stress** (the default) or **Pressure**. Then enter a value or expression for the **Normal stress** f_0 (SI unit: $\mathrm{N/m^2}$) or **Pressure** p_0 (SI unit: Pa). The defaults are 1 atm for both. For **Normal stress**, optionally enable **Suppress backflow**.

Periodic Condition

The **Periodic Condition** splits its selection into a source group and a destination group (the **Destination Selection** section is optional). It ensures that the flow and temperature fields at the source and destination boundaries are continuous. This corresponds to a situation where the geometry is a periodic part of a larger geometry. Flow characteristics at the boundary, described in Plane Wave Analysis of Inviscid Flow, are utilized to implement the continuity of the flow and temperature fields. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

BOUNDARY SELECTION

The software usually automatically identifies the boundaries as either source boundaries or destination boundaries, as indicated in the selection list. This works fine for cases like opposing parallel boundaries. In other cases, right-click **Periodic Condition** and select **Manual Destination Selection** to control the destination. By default it contains the selection that COMSOL Multiphysics identifies.

DESTINATION SELECTION

This section is available for specifying the destination boundaries, if needed, when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Condition** node. You can only select destination boundaries from the union of all source and destination boundaries.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping Between Source and Destination** section, see Mapping Between Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Symmetry

The **Symmetry** boundary condition prescribes no heat flux, no penetration and vanishing shear stresses. The boundary condition is a combination of Dirichlet conditions and a Neumann condition.

$$\mathbf{q}\cdot\mathbf{n}=\mathbf{0},\quad \mathbf{u}\cdot\mathbf{n}=\mathbf{0},\quad \left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=\mathbf{0}$$

Generate New Turbulence Model Interface

This global feature creates a new turbulent flow interface based on the current laminar or turbulent flow interface. The new interface inherits the property values from the original interface except for the turbulence related ones. All the features in the original interface are also inherited by the newly created interface except for the **Generate New Turbulence Model Interface** feature itself and the **Initial Values** feature. The initial values of the new interface are either default values or estimates from the solution of the original interface depending on the settings in the **Generate New Turbulence Model Interface** feature. Note that the parameters and expressions in text fields in all the features, except for **Initial Values** and the **Name** column in **Global Equation**, get exactly the same expressions as in the original model. Therefore, any dependencies on expressions or dependent variables from the physics interface must be reviewed and updated manually if necessary.

MODEL GENERATION

This section contains a Boolean input, **Copy only active settings**, which is selected by default. When selected, the disabled features and settings in the original model are not transferred to the new interface.

The **Create** button generates the new interface.

TURBULENCE MODEL INTERFACE

All available turbulence models can be selected from the list:

- The High Mach Number Flow, k-ε Interface
- The High Mach Number Flow, Algebraic yPlus Interface
- The High Mach Number Flow, L-VEL Interface
- The High Mach Number Flow, k-ω Interface
- The High Mach Number Flow, SST Interface
- The High Mach Number Flow, Low Reynolds Number k-ε Interface
- The High Mach Number Flow, Spalart–Allmaras Interface
- The High Mach Number Flow, v2-f Interface

- The High Mach Number Flow, Wilcox R-ω Interface
- The High Mach Number Flow, SSG-LRR Interface

STUDY

The **Study** section contains two lists: **Study type** and **Initial value from study**. When High Mach Number Flow, k-ε or High Mach Number Flow, k-ω is selected as the **Turbulence Model Interface**, the **Study type** contains the following two options:

- **Stationary**
- **Time-dependent**

The default value is **Stationary**. For all other turbulence models, the available **Study type** options are:

- **Stationary with initialization**
- **Time dependent with initialization**

with default value **Stationary with initialization**. Note that the created new study only solves for the new turbulence interface.

Initial value from study contains a list of the studies that are currently in the model. It can also be set to **None**. If there is no study available, the default option is **None**. If there are available studies, the first study is the default option.

These conditions correspond to the ones for the Single-Phase Flow, Laminar Flow interface. See Inlet and Outlet.

For a background on the derivation and implementation of the conditions, see Theory for the High Mach Number Flow Interfaces.

Selecting appropriate outlet conditions for the Navier–Stokes equations is not a trivial task. Generally, if there is something interesting happening at an outflow boundary, extend the computational domain to include this phenomenon.

The Compressible Euler Equations Interface

The **Compressible Euler Equations (cee)** interface ( ), found under the **Fluid Flow** > **High Mach Number Flow** branch ( ) when adding a physics interface, is used to model transient isentropic gas flows where the velocity magnitude is comparable to the speed of sound, that is, compressible flows in the transonic and supersonic range. This state is often connected to very low pressures.

The interface is based on the discontinuous Galerkin method (DG-FEM) and uses a time-explicit solver. The method is very memory lean. The physics interface solves for conservation of mass, momentum, and energy, neglecting dissipative effects. The dependent variables are the density, momentum, and total energy. Simulations using the **Compressible Euler Equations** interface are always time dependent.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Initial Values**, and **Wall**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the **Compressible Euler Equations** node to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `cee`.

PHYSICAL MODEL

When the **Include gravity** checkbox is selected, a global Gravity feature is shown in the interface model tree, and the buoyancy force is included in the Euler equations.

NUMERICAL FLUX

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Select the Numerical flux — **Lax-Friedrichs** (the default) or **Osher-Solomon Riemann solver**.

LIMITER

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog. Normally these settings do not need to be changed. Note that these settings are ignored when the discretization is set to **Constant**.

If the **WENO** limiter is selected from the **Limiter** list, the following settings are available:

- Choose the **Trouble cell indicator**: **TVB** (default) or **Off**. If TVB is selected, provide a **TVB constant** (default: 10). The TVB method is used to limit the elements where the WENO limiter is applied. This will reduce the cost of the limiter. A larger value of the TVB constant means that a smaller number of cells will use WENO.
- Select the **Positivity-preserving limiter for density and pressure** checkbox to maintain the positivity of pressure and density and prevent numerical blow-ups.

Shock Capturing and Positivity-Preserving Limiters

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Select the **CFL number**. This CFL number will be used when defining the **Cell time scale expression** `cee.wtc` used in the **Time-Explicit Solver** if the **Time stepping** is set to **From expressions**. Note that the method will be unstable for CFL numbers larger than 1.

In the *COMSOL Multiphysics Reference Manual*:

- References for the Solution Operation Nodes and Solvers

DISCRETIZATION

In this section you can select the order of the shape function of the dependent variables. The Compressible Euler Equations interfaces uses **Nodal discontinuous Lagrange** functions. Select the **Element order** — **Linear** (default) or **Constant**.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Density** rho (SI unit: kg/m^3), the **Momentum** m (SI unit: $kg/(m^2 \cdot s)$), and the **Total energy** etot (SI unit: J/m^3). The names can be changed but the names of fields and dependent variables must be unique within a component.

Theory for the Compressible Euler Equations Interface

Domain, Boundary, Edge, Point, and Pair Nodes for the Compressible Euler Equations Interface

The following nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users):

- Continuity
- Fluid Properties
- Gravity
- Heat Source
- Initial Values
- Inlet
- Interior Wall
- Outlet
- Symmetry
- Volume Force
- Wall

For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

The **Fluid Properties** node adds the continuity, momentum, and energy equations solved by the physics interface, except for volume forces and heat sources, which are added by the Volume Force and Heat Source features. Gravity is added by a global Gravity feature when **Include gravity** is selected in the **Physical Model** settings. The **Fluid Properties** node also provides settings for defining the material properties of the fluid.

THERMODYNAMICS

The Compressible Euler Equations interface is applicable for ideal gases. Specify the thermodynamics properties by selecting a ratio of specific heats and selecting between entering the specific gas constant, the heat capacity at constant pressure, or the mean molar mass. For an ideal gas the density is defined as

$$\rho = \frac{M_n p_A}{RT} = \frac{p_A}{R_s T}$$

where p_A is the absolute pressure, and T is the temperature.

Enter a value for the **Ratio of specific heats** γ (dimensionless). The ratio of specific heats must be a real number larger than 1.

Select a **Gas constant type** — **Specific gas constant** R_s (SI unit: J/(kg·K)), **Heat capacity at constant pressure** C_p (SI unit: J/(kg·K)), or **Mean molar mass** M_n (SI unit: kg/mol). The default setting is to use the property value **From material**. For **User defined** enter another value or expression for either material property. For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K), which is a built-in physical constant, is also used.

Initial Values

The **Initial Values** node adds initial values for the transient simulation.

INITIAL VALUES

You can provide initial values for the **Primitive Variables** (default) or **Conservative Variables**.

- If **Primitive Variables** is selected, provide a value for the density ρ (SI unit: kg/m^3), velocity $\mathbf{u}$ (SI unit: m/s), and pressure p (SI unit: Pa).
- If **Conservative Variables** is selected, provide a value for the density ρ (SI unit: kg/m^3), momentum $\mathbf{m}$ (SI unit: kg/(m^2 s), and total energy e (SI unit: J/m^3).

Volume Force

The **Volume Force** node specifies the volume force $\mathbf{F}$ on the right-hand side of the momentum equation, and a source term on the right-hand side of the energy equation.

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla \cdot [\rho(\mathbf{u} \otimes \mathbf{u}) + p\mathbf{I}] = \mathbf{F}$$

$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot [(e_{tot} + p)\mathbf{u}] = \mathbf{F} \cdot \mathbf{u}$$

If several volume-force nodes are added to the same domain, then the sum of all contributions are added to the momentum and energy equations.

VOLUME FORCE

Enter a value for the volume force $\mathbf{F}$ (SI unit: $\mathrm{N/m^3}$).

Heat Source

This node describes heat generation within the domain. Express heating and cooling with positive and negative values, respectively. Add one or more nodes as needed — all heat sources within a domain contribute to the total heat source.

A source term Q is added to the right-hand side of the energy equation.

$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot [(e_{tot} + p)\mathbf{u}] = Q$$

HEAT SOURCE

Enter a value for the heat source Q (SI unit: $\mathrm{W/m^3}$).

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at walls. A no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, is enforced. Since viscous effects are neglected, no boundary layer develops.

The no-penetration condition is imposed weakly setting the following flux:

$$\Gamma_\rho \cdot \mathbf{n} = 0$$

$$-\Gamma_m \cdot \mathbf{n} = p\mathbf{n}$$

$$\Gamma_e \cdot \mathbf{n} = 0$$

Theory for the Compressible Euler Equations Interface

Inlet

This condition provides the fluxes to describe the flow conditions at an inlet. The applied conditions are controlled by the **Flow Condition**.

This condition uses the Osher-Solomon Riemann Solver (Ref. 4) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW CONDITION

Select a **Flow condition** — **Supersonic** (the default) or **Subsonic**.

- For **Subsonic**, a subsonic ($Ma < 1$) inlet is specified. The imposed flux uses the imposed density and velocity, and computes the pressure from the interior of the domain.
- For **Supersonic** the inlet flow is assumed to be supersonic ($\mathrm{Ma} > 1$). A full set of variables must be provided in **Flow Properties**. The numerical flux can determine which characteristics are entering and leaving the domain, and can use values from inside the domain when the condition requires it.

In transonic flows ($0.8 < \mathrm{Ma} < 1.2$), or in cases where the flow may range from subsonic to supersonic, it is safer to use the **Supersonic** condition and let the characteristics based method determine the values used when computing the inlet flux.

FLOW PROPERTIES

Specify the flow properties at the inlet. If the inlet is **Subsonic**, enter values or expressions for the **Static density** $\rho_{0,\mathrm{stat}}$ (SI unit: Pa) and **Velocity** $\mathbf{u}_0$ (SI unit: m/s).

In **Supersonic** inlets, the inlet can be specified in terms of primitive variables, conservative variables, or a combination of static or total primitive variables and Mach

number. Select an **Input state** — **Primitive variables** (the default), **Conservative variables**, **Static state**, or **Total state**.

- For **Primitive variables** enter values or expressions for the **Static density** $\rho_{0,\mathrm{stat}}$ (SI unit: $\mathrm{kg/m^3}$), **Velocity** $\mathbf{u}_0$ (SI unit: m/s), and **Static pressure** $p_{0,\mathrm{stat}}$ (SI unit: Pa).
- For **Conservative variables** enter values or expressions for the **Static density** $\rho_{0,\mathrm{stat}}$ (SI unit: $\mathrm{kg/m^3}$), **Momentum** $\mathbf{m}_0$ (SI unit: $\mathrm{kg/(m^2\ s)}$, and **Total energy** e_{tot} (SI unit: $\mathrm{J/m^3}$).
- For **Static state** enter values or expressions for the **Static pressure** $p_{0,\mathrm{stat}}$ (SI unit: Pa), **Static temperature** $T_{0,\mathrm{stat}}$ (SI unit: K), and **Mach number** Ma_0 (dimensionless).
- For **Total state** enter values or expressions for the **Total pressure** $p_{0,\mathrm{tot}}$ (SI unit: Pa) and **Total temperature** $T_{0,\mathrm{tot}}$ (SI unit: K), and **Mach number** Ma_0 (dimensionless).

The relationships between the static and total states are:

$$\frac{p_{\mathrm{tot}}}{p_{\mathrm{stat}}} = \left(1 + \frac{\gamma - 1}{2}\mathrm{Ma}^2\right)^{\frac{\gamma}{\gamma - 1}}$$
$$\frac{T_{\mathrm{tot}}}{T_{\mathrm{stat}}} = \left(1 + \frac{\gamma - 1}{2}\mathrm{Ma}^2\right) \tag{5-3}$$

Select a **Flow direction** — **Normal inflow** (the default) or **User defined** to specify an arbitrary flow direction. Then enter the components of the direction normal n_{M} (dimensionless).

Outlet

This condition provides the fluxes to describe the flow conditions at an outlet. The applied conditions are controlled by the **Flow Condition**.

This condition uses the Osher-Solomon Riemann Solver (Ref. 4) to determine the incoming and outgoing characteristics, and provide the appropriate flux.

FLOW CONDITION

Select a **Flow condition** — **Subsonic** (the default) or **Supersonic**.

- For **Subsonic**, a subsonic ($\mathrm{Ma} < 1$) outlet is specified. The imposed flux computes the density and velocity from inside the domain, and uses the pressure specified in **Flow Properties**.
- For **Supersonic** the outlet flow is assumed to be supersonic ($\mathrm{Ma} > 1$). All the characteristics are assumed to be leaving the domain, and no variable needs to be specified.

In transonic flows ($0.8 < \mathrm{Ma} < 1.2$) or in cases where the flow may range from subsonic to supersonic, it is safer to use the **Subsonic** condition and let the characteristics based method determine the values used when computing the outlet flux.

FLOW PROPERTIES

This section is available when **Subsonic** is selected. Enter a value or expression for the **Static pressure** $p_{0,\mathrm{stat}}$ (SI unit: Pa).

Symmetry

The **Symmetry** boundary condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$.

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at $r = 0$. The software automatically provides an **Axial Symmetry** node prescribing $\mathbf{u} \cdot \mathbf{n} = 0$ on the axial symmetry boundaries.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall condition can be used to avoid meshing thin structures by applying a no-penetration condition on interior curves and surfaces instead.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the Wall node is used as fallback unless another feature has been selected for the boundary.

About Pairs

Gravity

The **Gravity** global feature is automatically added when **Include Gravity** is selected at the interface level in the **Physical Model** settings. A volume force and a source term are added on the right-hand side of the momentum and energy equations, respectively.

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot [\rho(\mathbf{u} \otimes \mathbf{u}) + p\mathbf{I}] = \rho \mathbf{g}$$

$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot [(e_{tot} + p)\mathbf{u}] = \rho \mathbf{g} \cdot \mathbf{u}$$

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s^2, default value $-g_{const}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{const}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

The Rotating Machinery, High Mach Number Flow Interfaces

The **Rotating Machinery, High Mach Number Flow** branch, found under the **Fluid Flow** > **High Mach Number Flow** branch (), contains three variations of the same predefined multiphysics interface (all with the name `hmnf`) for modeling gas flows where one or more of the boundaries rotate in a periodic fashion and the velocity magnitude is comparable to the speed of sound in the gas; that is, it flows in the transonic and supersonic range. The **High Mach Number Flow, Laminar** () and **High Mach Number Flow, Turbulent** () versions can be found under the **High Mach Number Flow** > **Rotating Machinery, High Mach Number Flow** branch (), when adding a physics interface. The physics interfaces can be used to model high-speed turbomachinery equipment.

The physics interfaces support **Sutherland's law** for **Thermal conductivity** and **Dynamic viscosity** as the default option.

In this chapter:

- Rotating Machinery, High Mach Number Flow, Laminar Flow Interface
- Rotating Machinery, High Mach Number Flow, k-ε Interface
- Rotating Machinery, High Mach Number Flow, Spalart–Allmaras Interface

Rotating Machinery, High Mach Number Flow, Laminar Flow Interface

The **Laminar Flow** version of the **Rotating Machinery, High Mach Number Flow (hmnf)** interface (), found under the **High Mach Number Flow** > **Rotating Machinery, High Mach Number Flow** branch (), is used to simulate gas flows in geometries with one or more rotating parts and gas at low and moderate Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, laminar flows in the transonic and supersonic range. This state is often connected to very low pressures. The physics interface is available for 3D and 2D components and it combines the **High Mach Number Flow, Laminar** interface (), with a **Rotating Domain** under **Definitions** > **Moving Mesh**.

There are two study types available for this physics interface. Using the **Time Dependent** study type, rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and rotation is accounted for by the inclusion of centrifugal and Coriolis forces. In both types, the physics interface solves for conservation of energy, mass, and momentum. The physics interface also supports heat transfer in solids as well as surface-to-surface radiation. However, only fluid domains adjacent to pair boundaries are supported.

When this multiphysics interface is added, the following default nodes are also added in the **Model Builder** under **High Mach Number Flow, Laminar** — **Fluid**, **Initial Values**, **Wall**, and **Thermal Insulation**. When a pair boundary is created, the **Continuity** node is automatically added. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu. See Moving Mesh for more details on the **Rotating Domain** node added automatically in the **Model Builder** under **Definitions** > **Moving Mesh**.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `hmnf`.

PHYSICAL MODEL

The **Reference temperature** T_{ref} is used to define the reference enthalpy H_{ref} which is set to 0 J/kg at p_{ref} (1 atm) and T_{ref}. When the **Include kinetic energy** checkbox is selected, the conservative total-energy equation is solved.

TURBULENCE

Turbulence Model Type

By definition, no turbulence model is needed when studying laminar flows. The default is **None**.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). The names can be changed but the names of fields and dependent variables must be unique within a component.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** checkbox to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** calculates the local CFL number (from the Courant–Friedrichs–Lewy condition) from a built-in expression. For **Manual** enter a **Local CFL number** $\mathrm{CFL}_{\mathrm{loc}}$.

By default the **Enable conversions between material and spatial frames** checkbox is selected.

Rotating Machinery, High Mach Number Flow, k-ε Interface

The **Turbulent Flow, k-ε** version of the **Rotating Machinery, High Mach Number Flow (hmnf)** interface ( ), found under the **High Mach Number Flow** > **Rotating Machinery, High Mach Number Flow** > **Turbulent Flow** branch ( ), is used to simulate gas flows in geometries with one or more rotating parts and gas at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range. The physics interface is available for 3D and 2D components and it combines the **High Mach Number Flow, k-ε** interface ( ), with a **Rotating Domain** under **Definitions** > **Moving Mesh**.

There are two study types available for this physics interface. Using the **Time Dependent** study type, rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and rotation is accounted for by the inclusion of centrifugal and Coriolis forces. In both types, the physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow and heat transfer close to walls are modeled using wall functions. The physics interface also supports heat transfer in solids as well

as surface-to-surface radiation. However, only fluid domains adjacent to pair boundaries are supported.

When this multiphysics interface is added, the following default nodes are also added in the **Model Builder** under **High Mach Number Flow, k-ε** — **Fluid**, **Initial Values**, **Wall**, and **Thermal Insulation**. When a pair boundary is created, the **Continuity** node is automatically added. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu. See Moving Mesh for more details of the **Rotating Domain** node added automatically in the **Model Builder** under **Definitions** > **Moving Mesh**.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `hmnf`.

PHYSICAL MODEL

The **Reference temperature** T_{ref} is used to define the reference enthalpy H_{ref} which is set to 0 J/kg at p_{ref} (1 atm) and T_{ref}. When the **Include kinetic energy** checkbox is selected, the conservative total-energy equation is solved.

TURBULENCE

The default **Turbulence model type** is **RANS**, the default **Turbulence model** is **k-ε**, and the default **Heat transport turbulence model** is **Kays–Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the **Fluid** node.

Edit Turbulence Model Parameters

Edit the model parameters of the k-ε model as needed. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the

turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling, **Turbulent kinetic energy** k (SI unit: m^2/s^2) and **Turbulent dissipation rate** ep (SI unit: m^2/s^3) variables are also available.

The names can be changed but the names of fields and dependent variables must be unique within a model.

Rotating Machinery, High Mach Number Flow, Spalart–Allmaras Interface

The **Turbulent Flow, Spalart-Allmaras** version of the **Rotating Machinery, High Mach Number Flow (hmnf)** interface ( ), found under the **High Mach Number Flow** > **Rotating Machinery, High Mach Number Flow** > **Turbulent Flow** branch ( ), is used to simulate

gas flows in geometries with one or more rotating parts and gas at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.The physics interface is available for 3D and 2D components and it combines the **High Mach Number Flow, Spalart-Allmaras** interface ( ), with a **Rotating Domain** under **Definitions** > **Moving Mesh**.

There are two study types available for this physics interface. Using the **Time Dependent** study type, rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and rotation is accounted for by the inclusion of centrifugal and Coriolis forces. Turbulence effects are modeled using the one-equation Spalart-Allmaras turbulence model. The Spalart-Allmaras model is a so-called low-Reynolds number model, which means that it resolves the velocity, pressure, and temperature fields all the way down to the wall. The Spalart-Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation. A **Wall Distance Initialization** study type is automatically added. It also supports heat transfer in solids as well as surface-to-surface radiation. However, only fluid domains adjacent to pair boundaries are supported.

When this multiphysics interface is added, the following default nodes are also added in the **Model Builder** under **High Mach Number Flow, Spalart-Allmaras** — **Fluid**, **Initial**

Values, **Wall**, and **Thermal Insulation**. When a pair boundary is created, the **Continuity** node is automatically added. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu. See Moving Mesh for more details of the **Rotating Domain** node added automatically in the **Model Builder** under **Definitions** > **Moving Mesh**.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `hmnf`.

PHYSICAL MODEL

The **Reference temperature** T_{ref} is used to define the reference enthalpy H_{ref} which is set to 0 J/kg at p_{ref} (1 atm) and T_{ref}. When the **Include kinetic energy** checkbox is selected, the conservative total-energy equation is solved.

TURBULENCE

The default **Turbulence model type** is **RANS**, the default **Turbulence model** is **Spalart-Allmaras**, and the default **Heat transport turbulence model** is **Kays–Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the **Fluid** node.

Edit Turbulence Model Parameters

Edit the model parameters of the Spalart–Allmaras model as needed. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling, **Reciprocal wall distance** G (SI unit: 1/m) and **Undamped turbulent kinematic viscosity** nutilde (SI unit: m^2/s) variables are also available.

The names can be changed but the names of fields and dependent variables must be unique within a model.

Theory for the High Mach Number Flow Interfaces

In some industrial applications involving fluid flow, the flow velocity is large enough to introduce significant changes in the density and temperature of the fluid. This occurs because the thermodynamic properties of the fluid are coupled. Appreciable changes in the fluid properties are encountered as the flow velocity approaches, or exceeds, the speed of sound. As a rule of thumb, velocities greater than 0.3 times the speed of sound are considered to be *high Mach number* flows.

The High Mach Number Flow interface theory is described in this section:

- Compressible Flow for All Mach Numbers
- Sutherland's Law
- Consistent Inlet and Outlet Conditions
- Pseudo Time Stepping for High Mach Number Flow Models
- References for the High Mach Number Flow Interfaces

Compressible Flow for All Mach Numbers

The High Mach Number Flow interfaces solve the following equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{5-4}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} \tag{5-5}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T \right) = -(\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T}\bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p \right) + Q \tag{5-6}$$

where

- ρ is the density (SI unit: $\mathrm{kg/m^3}$)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is the pressure (SI unit: Pa)
- τ is the viscous stress tensor (SI unit: Pa)

- $\mathbf{F}$ is the volume force vector (SI unit: $\mathrm{N/m^3}$)
- C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- $\mathbf{q}$ is the heat flux vector (SI unit: $\mathrm{W/m^2}$)
- Q contains the heat sources (SI unit: $\mathrm{W/m^3}$)
- $\mathbf{S}$ is the strain-rate tensor:

$$\mathbf{S} = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

When, in addition, the **Include kinetic energy** checkbox is selected, the conservative total-energy equation is solved

$$\frac{\partial}{\partial t}\left[\rho\left(e + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] + \nabla\cdot\left[\rho\mathbf{u}\left(h + \frac{1}{2}\|\mathbf{u}\|^2\right)\right] = \nabla\cdot(\mathbf{u}\cdot\tau - \mathbf{q}) + Q \tag{5-7}$$

where

$$h = h(T_{\mathrm{ref}}, p_{\mathrm{ref}}) + \int_{T_{\mathrm{ref}}}^{T} C_p dT + \int_{p_{\mathrm{ref}}}^{p} \frac{(1-\alpha_p T)}{\rho} dp, \quad e = h - \frac{p}{\rho} \tag{5-8}$$

These are the fully compressible Navier-Stokes equations for a simple compressible fluid. As can be seen, the same set of equations can be assembled using, for example, a Nonisothermal Flow interface or by manually coupling a Single-Phase Flow interface with a Heat Transfer interface. The difference is that the High Mach Number Flow interface can handle flow of any Mach numbers, while the other physics interfaces are subject to The Mach Number Limit. The Mach number is defined as

$$\mathrm{Ma} = \frac{|\mathbf{u}|}{a}$$

where a is the speed of sound. Equation 5-4 is hyperbolic whereas Equation 5-5 and Equation 5-6 are parabolic for time-dependent flow and elliptic for stationary flow. If diffusive effects can be neglected, as is usually the case for high-speed flows, the entire system of equations becomes hyperbolic. When the Mach number passes through unity, the direction of the characteristics associated with the hyperbolic system changes. This means that new phenomena not observed for incompressible flows, such as shock waves and expansion fans, can occur (Ref. 2). The stabilization and boundary conditions must be adapted to the change in direction of the characteristics.

Note that the diffusive effects do not disappear entirely unless these terms are explicitly excluded from the equations. Instead, they are confined to either boundary layers or to “shock-waves”, which are really thin regions with steep gradients. In the High Mach Number Flow interfaces these thin regions are assumed to be underresolved, and the stabilization takes this into account. If the details of these regions are of physical interest they must be adequately resolved.

The physics interface assumes that the fluid is an ideal gas. This is necessary for the formulation of the Consistent Inlet and Outlet Conditions. The ideal gas law relates density and specific heats to the pressure and temperature. The viscosity and thermal conductivity of an ideal gas can be accurately approximated using Sutherland’s Law, which is included as an option in the High Mach Number Flow interface.

The Mach Number Limit

Sutherland’s Law

Sutherland’s law, or Sutherland’s formula, is an approximation for how the viscosity of gases depends on the temperature. This law is based on an idealized intermolecular-force potential and reads (Ref. 5)

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2}\frac{T_0 + S_\mu}{T + S_\mu} \tag{5-9}$$

where S_μ is an effective temperature called the Sutherland constant. Each gas has its own Sutherland constant. Equation 5-9 is strictly valid only for single-component gases at low pressure. It does, however, work well for air because air is mainly composed of nitrogen and oxygen, which have very similar properties. Parameter values for some common gases are given in Table 5-2 (Ref. 5).

TABLE 5-2: SUTHERLAND’S LAW PARAMETERS FOR DYNAMIC VISCOSITY.

GAS	μ_0	T_0	S_μ
Air	$1.716\cdot10^{-5}$	273	111
Argon	$2.125\cdot10^{-5}$	273	114
$C0_2$	$1.370\cdot10^{-5}$	273	222
CO	$1.657\cdot10^{-5}$	273	136
N_2	$1.663\cdot10^{-5}$	273	107

TABLE 5-2: SUTHERLAND'S LAW PARAMETERS FOR DYNAMIC VISCOSITY.

GAS	μ_0	T_0	S_μ
O_2	$1.919 \cdot 10^{-5}$	273	139
H_2	$8.411 \cdot 10^{-6}$	273	97
Steam	$1.12 \cdot 10^{-5}$	350	1064

The SI unit for μ_0 in Table 5-2 is N·s/m^2. The SI unit for T_0 and S_μ is kelvin (K).

Sutherland's law can also be formulated for thermal conductivity (Ref. 5):

$$\frac{k}{k_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S_k}{T + S_k} \tag{5-10}$$

Values for k_0, T_0, and S_k for some common gases are given in Table 5-3(Ref. 5).

TABLE 5-3: SUTHERLAND'S LAW PARAMETERS FOR THERMAL CONDUCTIVITY.

GAS	k_0	T_0	S_k
Air	0.0241	273 K	194
Argon	0.0163	273	170
$C0_2$	0.0146	273	1800
CO	0.0232	273	180
N_2	0.0242	273	150
O_2	0.0244	273	240
H_2	0.168	273	120
Steam	0.0181	300	2200

The unit for k_0 in Table 5-3 is W/(m·K). The unit for T_0 and S_k is kelvin (K).

Consistent Inlet and Outlet Conditions

In order to provide consistent inlet and outlet conditions for high Mach number flow, the flow situation needs to be monitored at the boundary. Because all flow properties are coupled, the number and combinations of boundary conditions needed for *well posedness* depend on the flow state — that is, with which speeds the different flow quantities are propagated at the boundary. For a detailed specification on the number of physical boundary conditions needed for well posedness, see Ref. 1.

PLANE WAVE ANALYSIS OF INVISCID FLOW

On inlets a plane wave analysis of the inviscid part of the flow is used in order to apply a consistent number of boundary conditions. The method used here is described in Ref. 3.

Inviscid flow is governed by Euler's equations, which, provided that the solution is smooth and neglecting the gravity terms, can be written as

$$\frac{\partial Q}{\partial t} + \frac{\partial F_j}{\partial Q}\frac{\partial Q}{\partial x_j} = 0$$

Considering a small region close to a boundary, the Jacobian matrices can be regarded as constant, which leads to a system of linear equations

$$\frac{\partial Q}{\partial t} + \left(\frac{\partial F_j}{\partial Q}\right)_0 \frac{\partial Q}{\partial x_j} = 0$$

where the subscript 0 denotes a reference state at the boundary. Assuming that the state at the boundary, described by a unit surface normal vector $\mathbf{n}$ (pointing out from the domain), is perturbed by a plane wave, the linear system of equations can be transformed to

$$\frac{\partial Q}{\partial t} + A_0 \frac{\partial Q}{\partial \xi} = 0$$

where

$$A_0 = n_j \left(\frac{\partial F_j}{\partial Q}\right)_0$$

and ξ corresponds to the direction normal to the boundary. In the unsteady case, Euler's equations are known to be hyperbolic in all flow regimes: subsonic, sonic, and supersonic flow (Ref. 4). This implies that A_0 has real-valued eigenvalues and corresponding eigenvectors, and it can therefore be diagonalized according to

$$TA_0T^{-1} = \Lambda, \quad \Lambda_{ii} = \{\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5\}$$

The matrix T contains the (left) eigenvectors, and the matrix Λ is a diagonal matrix containing the eigenvalues. The eigenvalues are given exactly by

$$
\begin{aligned}
\lambda_1 &= n_i u_i \\
\lambda_2 &= \lambda_1 \\
\lambda_3 &= \lambda_1 \\
\lambda_4 &= \lambda_1 + c_s \\
\lambda_5 &= \lambda_1 - c_s
\end{aligned}
\tag{5-11}
$$

where c_s is the speed of sound. Using the primitive variables

$$
Q = \begin{bmatrix} \rho \\ u \\ v \\ w \\ p \end{bmatrix}
$$

The characteristic variables on the boundary are

$$
\begin{aligned}
w_1 &= \rho - \frac{p}{(c_s^A)^2} \\
w_2 &= \frac{n_1 v - n_2 u}{\sqrt{n_1 n_1 + n_2 n_2}} \\
w_3 &= w\sqrt{n_1 n_1 + n_2 n_2} - n_3\left(\frac{n_1 u + n_2 v}{\sqrt{n_1 n_1 + n_2 n_2}}\right) \\
w_4 &= \frac{1}{2}\left(\frac{\rho^A}{c_s^A}(n_i u_i) + \frac{p}{(c_s^A)^2}\right) \\
w_5 &= \frac{1}{2}\left(-\frac{\rho^A}{c_s^A}(n_i u_i) + \frac{p}{(c_s^A)^2}\right)
\end{aligned}
\tag{5-12}
$$

Each characteristic can be interpreted to describe a wave transporting some quantity. The first one is an entropy wave while the next two correspond to vorticity waves. The fourth and fifth, in turn, are sound waves.

Evaluating the primitive variables in Equation 5-12, the values are taken from the outside (specified values) or from the inside (domain values) depending on the sign of the eigenvalue corresponding to that characteristic variable. At inlets, a negative eigenvalue implies that the characteristic is pointing into the domain and hence outside values are used. Correspondingly, for a positive eigenvalue the inside values are used.

Variables in Equation 5-12 with a superscript A are computed as averages of the inside and outside values.

The characteristic variables are then transformed to consistent face values of the primitive variables on the boundary in the manner of

$$\begin{aligned}
\rho_b &= w_1 + w_4 + w_5 \\
u_{1,b} &= -\frac{n_2 w_2}{\sqrt{n_1 n_1 + n_2 n_2}} - n_1\left(\frac{n_3 w_3}{\sqrt{n_1 n_1 + n_2 n_2}} - \frac{c_s^A}{\rho^A}(w_4 - w_5)\right) \\
u_{2,b} &= \frac{n_1 w_2}{\sqrt{n_1 n_1 + n_2 n_2}} - n_2\left(\frac{n_3 w_3}{\sqrt{n_1 n_1 + n_2 n_2}} - \frac{c_s^A}{\rho^A}(w_4 - w_5)\right) \\
u_{3,b} &= w_3\sqrt{n_1 n_1 + n_2 n_2} + n_3\frac{c_s^A}{\rho^A}(w_4 - w_5) \\
p_b &= (c_s^A)^2(w_4 + w_5)
\end{aligned} \tag{5-13}$$

Characteristics Based Inlets

Applying this condition implies using the plane wave analysis described in Consistent Inlet and Outlet Conditions. With this condition, a varying flow situation at the inlet can be handled. This means that changes due to prescribed variations at the boundary, due to upstream propagating sound waves or spurious conditions encountered during the nonlinear solution procedure, can be handled in a consistent manner. The full flow condition at the inlet is specified by the following properties

$$M_{\text{in}}, p_{\text{in}}, T_{\text{in}} \tag{5-14}$$

from which the density is computed using the ideal gas law. The dependent variables defined in Equation 5-14 are applied as the outside values used in Equation 5-12, and the boundary values of the dependent variables are obtained from Equation 5-13.

Supersonic Inlets

Applying a supersonic inlet, the full flow at the inlet is specified using the inlet properties in Equation 5-14. Because the flow is supersonic, all characteristic at the inlet are known to be directed into the domain, and the boundary values of the dependent variables are computed directly from the inlet properties.

Subsonic Inlets

When the inlet flow is subsonic, it is possible to specify either the velocity or the pressure at the inlet. In either case, it is also necessary to either specify the temperature or a heat flux at the inlet. When a heat flux is specified, the following condition is applied,

$$k\nabla T \cdot \mathbf{n} = \rho C_p(T - T_{\text{ustr}})\min(\mathbf{u} \cdot \mathbf{n}, 0) \tag{5-15}$$

where T_{ustr} is the upstream temperature.

Hybrid Outlet

When building a model, it is recommended that it is constructed so that as little as possible happens at the outlet. In the high Mach number flow case this implies keeping the conditions either subsonic or supersonic at the outlet. This is, however, usually not possible. For example, often one boundary adjacent to the outlet consists of a no slip wall, in which case a boundary layer containing a subsonic region is present. The hybrid outlet feature adds the following weak expression:

$$\Gamma W_{\text{NS}} = \begin{cases} 0.5(-p - p_{\text{out}})\mathbf{n} \cdot \hat{\mathbf{u}} & Ma < 1 \\ (-p)\mathbf{n} \cdot \hat{\mathbf{u}} & \text{else} \end{cases}$$

where $\hat{\mathbf{u}}$ is the test function for the velocity vector. This corresponds to a pressure, no viscous stress condition in regions with subsonic flow and a no viscous stress condition in regions with supersonic flow. When the static pressure at the outlet is not known beforehand, it is recommended that it is set to the inlet pressure. When a converged solution has been reached, the solution can be analyzed to find the pressure level just outside the sonic point (Ma = 1) along the boundary. You can then apply this pressure level instead.

Supersonic Outlet

When the outlet condition is known to be fully supersonic, the viscous stress is specified in accordance with the equations and hence no physical condition is applied. This is done by prescribing the boundary stress using the full stress vector:

$$W_{\text{NS}} = \left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right](\mathbf{n} \cdot \hat{\mathbf{u}})$$

It is often possible to use the supersonic condition at outlets that are not strictly supersonic but mainly supersonic (the main part of the outlet boundary contains supersonic flow).

Pseudo Time Stepping for High Mach Number Flow Models

Pseudo time stepping is per default applied to all governing equations for stationary problems, for 2D component models as well as 3D component models. The momentum, continuity, energy, and turbulence equations (when present) use the same expression for the pseudo time step symbol $\Delta\tilde{t}$.

For laminar models the automatic expression for $\mathrm{CFL}_{\mathrm{loc}}$ is

$$\begin{aligned}&1 + \\ &\mathrm{if}(\mathrm{niterCMP} > 10,\ 1.2^{\min(\mathrm{niterCMP}-10,\ 12)},\ 0) + \\ &\mathrm{if}(\mathrm{niterCMP} > 32,\ 9 \cdot 1.3^{\min(\mathrm{niterCMP}-32,\ 9)},\ 0) + \\ &\mathrm{if}(\mathrm{niterCMP} > 60,\ 40 \cdot 1.3^{\min(\mathrm{niterCMP}-60,\ 9)},\ 0)\end{aligned}$$

while for models with turbulent flow it is

$$\begin{aligned}&1 + \\ &\mathrm{if}(\mathrm{niterCMP} > 10,\ 1.2^{\min(\mathrm{niterCMP}-10,\ 12)},\ 0) + \\ &\mathrm{if}(\mathrm{niterCMP} > 120,\ 1.3^{\min(\mathrm{niterCMP}-120,\ 9)},\ 0) + \\ &\mathrm{if}(\mathrm{niterCMP} > 220,\ 1.3^{\min(\mathrm{niterCMP}-220,\ 9)},\ 0)\end{aligned}$$

Pseudo Time Stepping for Laminar Flow Models

References for the High Mach Number Flow Interfaces

1. T. Poinsot and D. Veynante, *Theoretical and Numerical Combustion*, 2nd ed., Edwards, 2005.

2. J.D. Anderson, *Modern Compressible Flow*, 3rd ed., McGraw Hill, 2003.

3. J. Larsson, *Numerical Simulation of Turbulent Flows for Turbine Blade Heat Transfer Applications*, PhD thesis, Chalmers University of Technology, 1998.

4. J.D. Tannehill, D.A. Anderson, and R.H. Pletcher, *Computational Fluid Mechanics and Heat Transfer*, 2nd ed., Taylor & Francis, 1997.

5. F.M. White, *Viscous Fluid Flow*, 3rd ed., McGraw Hill, 2006.

Theory for the Compressible Euler Equations Interface

In this section:

- The Compressible Euler Equations
- The Numerical Method
- Shock Capturing and Positivity-Preserving Limiters
- References for the Compressible Euler Equations Interface

The Compressible Euler Equations

The Euler equations form a set of hyperbolic equations governing inviscid and adiabatic flow. The Compressible Euler Equations interface solves the transient compressible version of the Euler equations for ideal gases

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{5-16}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot [\rho(\mathbf{u} \otimes \mathbf{u}) + p\mathbf{I}] = \mathbf{F} + \rho \mathbf{g} \tag{5-17}$$

$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot [(e_{tot} + p)\mathbf{u}] = Q + \mathbf{F} \cdot \mathbf{u} + \rho \mathbf{g} \cdot \mathbf{u} \tag{5-18}$$

where

- ρ is the density (SI unit: $\mathrm{kg/m^3}$)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- $\rho\mathbf{u}$ is the momentum vector (SI unit: $\mathrm{kg/(m^2\ s)}$)
- p is the absolute pressure (SI unit: Pa)
- e_{tot} is the total energy (SI unit: $\mathrm{J/m^3}$)
- $\mathbf{F}$ is the volume force vector (SI unit: $\mathrm{N/m^3}$)
- Q is the volumetric heat source (SI unit: $\mathrm{W/m^3}$)
- $\mathbf{g}$ is the acceleration of gravity (SI unit: $\mathrm{m/s^2}$)
- $\mathbf{I}$ is the identity matrix

The volume force and heat source terms can be added using the Volume Force and Heat Source features, respectively. The gravity terms are added when **Include Gravity** is selected at the interface level in the **Physical Model** settings.

The physics interface assumes that the fluid is an ideal gas. This is used in the definition of the Inlet and Outlet fluxes and the positivity-preserving limiter (see Shock Capturing and Positivity-Preserving Limiters). The equation of state for the internal energy per unit volume e is

$$e = \frac{p}{\gamma - 1}$$

Where γ is the ratio of specific heats (dimensionless), which is assumed constant. The total energy is expressed as the sum of the internal energy and the kinetic energy

$$e_{tot} = \frac{p}{\gamma - 1} + \frac{1}{2}\rho \mathbf{u}^2$$

The physics interface solves for the conservative dependent variables, which are the density, momentum, and total energy. In some features, the primitive variables, density, velocity, and pressure, may be used to impose initial or boundary conditions.

The absolute temperature T (SI unit: K) can be obtained from the equation of state for an ideal gas

$$T = \frac{p}{R_s \rho}$$

where R_s is the specific gas constant (SI unit: J/(kg·K)).

The Numerical Method

The physics interface solves the compressible Euler equations using the Discontinuous Galerkin (DG) method in space together with explicit time stepping. The computations are restricted to transient problems. The basis functions are the nodal discontinuous Lagrange shape functions.

The numerical method used solves wave problems of the form

$$\mathbf{d}_a \frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \Gamma(\mathbf{w}) = \mathbf{f}$$

In the compressible Euler equations, $\mathbf{d}_a$ is an identity matrix, $\mathbf{w}$ is the vector of conservative variables, Γ represents the conservative fluxes, and $\mathbf{f}$ includes the volumetric forces, heat sources, and gravity terms:

$$\mathbf{w} = \begin{bmatrix} \rho \\ \rho\mathbf{u} \\ e_{\text{tot}} \end{bmatrix}$$

$$\Gamma(\mathbf{w}) = \begin{bmatrix} \Gamma_\rho \\ \Gamma_m \\ \Gamma_e \end{bmatrix} = \begin{bmatrix} \rho\mathbf{u}^T \\ \rho(\mathbf{u}\otimes\mathbf{u}) + p\mathbf{I} \\ (e_{\text{tot}} + p)\mathbf{u}^T \end{bmatrix}$$

$$\mathbf{f} = \begin{bmatrix} 0 \\ \mathbf{F} + \rho\mathbf{g} \\ Q + \mathbf{F}\cdot\mathbf{u} + \rho\mathbf{g}\cdot\mathbf{u} \end{bmatrix}$$

Here, Γ_ρ, Γ_m, and Γ_e represent the fluxes of the continuity, momentum, and energy equations, respectively.

Discontinuous Galerkin methods use shape functions that are continuous in the interior of each mesh element, but discontinuous across the element boundaries. A numerical flux must be defined across element boundaries, and the dependent variables are not required to be continuous on faces between adjacent mesh elements. The default numerical flux is the Lax-Friedrichs flux, which uses an average of the physical fluxes together with a penalty term. The Osher–Solomon flux is also available (see Ref. 4).

After discretization in space, the system of equations is integrated in time. The standard procedure is to use an explicit Runge–Kutta method. The physics interface uses the third-order SSP (strong stability preserving) Runge–Kutta method per default.

The time step in explicit computations is limited by the CFL condition; see Time Explicit Integrator in the *COMSOL Multiphysics Reference Manual*. The maximum stable time step is proportional to the smallest mesh element size h, and inversely proportional to the maximum wave speed in the domain. On unstructured meshes with local refinement regions only a few elements are small, yet these dictate the overall time step for the whole problem. In such cases, the use of Local Time Stepping is

advisable. COMSOL Multiphysics provides the **Adams-Bashforth 3 (local)** time stepping method.

Theory for the Wave Form PDE in the *COMSOL Multiphysics Reference Manual*.

Shock Capturing and Positivity-Preserving Limiters

The compressible Euler equations form a system of hyperbolic conservation laws that can develop discontinuous solutions even starting from a continuous initial solution. These discontinuous solutions appear in the form of shock waves or contact waves, and induce spurious oscillations and instabilities in the numerical solution when shape functions other than constant are used. The control of oscillations around discontinuities requires the use of a limiter to preserve the order of accuracy and achieve sharp, nonoscillatory solutions.

The compressible Euler equations interface includes a *weighted essentially nonoscillatory* (WENO) limiter for use in the discontinuous Galerkin method, which is applied in each inner stage of the time-explicit solver. The WENO limiter reconstructs the polynomial of the DG solution in a troubled element from a convex combination of the polynomials in the current element and its immediate neighbors based on smoothness indicators and nonlinear weights, and includes adjustments to guarantee conservation. A *total variation bounded* (TVB) troubled cell indicator is available to limit the use of WENO to the elements where it is needed and reduce computational costs. The TVB constant can be set by the user and a larger value means that a smaller number of elements will use WENO. For more information on the WENO limiter, see Ref. 2.

The compressible Euler equations are well posed only if both density and pressure are positive. When using constant interpolations, the positivity of density and pressure is guaranteed if the CFL condition for the time step is satisfied. If the dependent variables are discretized with linear shape functions, the positivity of density and pressure is not ensured even when satisfying the CFL condition and using the WENO limiter. Therefore, the physics interface includes a positivity-preserving limiter for density and pressure which can be used together with WENO to prevent numerical blow-ups. See Ref. 3 for more information.

References for the Compressible Euler Equations Interface

1. J.D. Anderson, *Modern Compressible Flow*, 3rd ed., McGraw Hill, 2003.

2. J. Zhu, X. Zhong, C.W. Shu, and J. Qiu, "Runge–Kutta discontinuous Galerkin method using a new type of WENO limiters on unstructured meshes," *J. Comput. Phys.*, vol. 248, pp. 200–220, 2013.

3. X. Zhang, Y. Xia, and C.W. Shu, "Maximum-principle-satisfying and positivity-preserving high order discontinuous Galerkin schemes for conservation laws on triangular meshes," *J. Sci. Comput.*, vol. 50, no. 1, pp. 29–62, 2012.

4. J. Felcman and P. Šolín, "On the Construction of the Osher–Solomon Scheme for 3D Euler Equations, East–West," *J. Num. Math.*, vol. 6, pp. 43–64, 1998.

6

Multiphase Flow Interfaces

This chapter discusses the physics interfaces found under the **Fluid Flow** > **Multiphase Flow** branch ( ). The section Modeling Multiphase Flow helps you choose the best physics interface to start with.

In this chapter:

- The Two-Phase Flow, Level Set and Phase Field Interfaces
- The Two-Phase Thin-Film Flow, Phase Field Interfaces
- The Three-Phase Flow, Phase Field Interface
- The Laminar Two-Phase Flow, Moving Mesh Interface
- The Bubbly Flow Interfaces
- The Mixture Model Interfaces
- The Euler–Euler Model Interfaces
- The Phase Transport Interfaces
- The Phase Transport Mixture Model Interfaces
- The Nonisothermal Mixture Model Interfaces
- Theory for the Two-Phase Flow Interfaces
- Theory for the Two-Phase Thin-Film Flow, Phase Field Interfaces

- Theory for the Three-Phase Flow Interface
- Theory for the Two-Phase Flow, Moving Mesh Interface
- Theory for the Bubbly Flow Interfaces
- Theory for the Mixture Model Interfaces
- Theory for the Euler–Euler Model Interfaces
- Theory for the Phase Transport Interfaces
- Theory for the Phase Transport Mixture Model Interfaces
- Theory for the Nonisothermal Mixture Model Interfaces

Modeling Multiphase Flow

In this section:

- Selecting the Right Physics Interface
- The Multiphase Flow Interface Options
- The Relationship Between the Physics Interfaces
- Coupling to Other Physics Interfaces

Certain types of multiphase flow can be described using the Phase Field in Fluids and Level Set interfaces found under the **Mathematics>Moving Interface** branch ( ).

- The Physics Interfaces in the *COMSOL Multiphysics Reference Manual*
- Mathematics, Moving Interface Branch

Selecting the Right Physics Interface

The **Multiphase Flow** branch ( ) included with this module has a number of subbranches to describe momentum transport for multiphase flow. One or more physics interfaces can be added; either singularly or in combination with other physics interfaces for applications such as mass transfer and energy (heat) transfer.

Different types of flow require different equations to describe them. If you know the type of flow to model, then select it directly. However, when you are not certain of the flow type, or when it is difficult to obtain a solution, you can instead start with a simplified model and add complexity as you build the model. Then you can successively advance forward, comparing models and results.

The Bubbly Flow, Mixture Model, Euler-Euler Model, and Phase Transport Mixture Model interfaces are appropriate when you want to simulate a flow with many particles, droplets, or bubbles immersed in a liquid. With these physics interfaces, you do not track each particle in detail. Instead you solve for the averaged volume fraction. If you are interested in the exact motion of individual bubbles, including how the fluid

interface deforms due to, for instance, surface tension, use any of the Two-Phase Flow interfaces.

To model the detailed dynamics of fluid interfaces, either use the level set method, the phase field method, the phase field thin-film flow method, or by a moving mesh, respectively. For problems involving topological changes (for example, jet breakup), use either the Level Set, Phase Field in Fluids or Phase Field Thin-Film Flow interfaces.These techniques use an auxiliary function (the level set and phase field functions, respectively) to track the location of the interface, which is necessarily diffuse. The Level Set interface does not include the surface tension force per default, and is recommended for use in large scale problems dominated by inertia, or when the effects of the gradient of the surface tension coefficient are relevant. The phase field method is physically motivated and is usually more numerically stable than the level set method. It is can also be extended to more phases and is compatible with fluid-structure interactions (requires the MEMS Module or the Structural Mechanics Module). In general, it is not obvious which one of these to use when the flow is convection dominated. However, when the flow is diffusion dominated, for example, in the case of phase separation, the phase field method should be used. Phase Field Thin-Film Flow method may be used to track the location of the interface in narrow channels, represented by a surface or an edge within the geometry, which are thin enough for the Reynolds equation or the modified Reynolds equation to apply.

The flow of two immiscible fluids in narrow channels can be simulated using the Two-Phase Thin-Film Flow, Phase Field interfaces.

The moving mesh method represents the interface as a boundary condition along a line or surface in the geometry. Because the physical thickness of phase boundaries is usually very small, for most practical meshes The Laminar Two-Phase Flow, Moving Mesh Interface describes the two-phase boundary more accurately. However, it cannot accommodate topological changes in the boundary.

Three-phase flow can be simulated using the Laminar Three-Phase Flow, Phase Field interface.

The Multiphase Flow Interface Options

For any of the Multiphase Flow interfaces, except for the Two-Phase Thin-Film Flow, Phase Field interfaces, you can assume either laminar or turbulent flow as the starting point. This enables you to make the appropriate mathematical model assumptions required to solve the flow.

The Relationship Between the Physics Interfaces

Several of the interfaces vary only by one or two default settings (see Table 6-1, Table 6-2, Table 6-4, and Table 6-5) in the **Physical Model** and **Turbulence** sections, which are selected either from a checkbox or a list. For the **Multiphase Flow** branch, the **Bubbly Flow (bf)**, **Mixture Model (mm)**, **Euler-Euler Model (ee)**, and **Phase Transport** subbranches have several physics interfaces each depending on the turbulence model used. All the Two-Phase Flow interfaces contain a multiphysics coupling feature with a name as (tpf). The **Three-Phase Flow, Phase Field** branch contains a single interface for laminar flow.

BUBBLY FLOW

TABLE 6-1: BUBBLY FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	LOW GAS CONCENTRATION	TURBULENT MODEL TYPE	TURBULENT MODEL	SOLVE FOR INTERFACIAL AREA
Laminar Bubbly Flow	bf	Yes	None	n/a	No
Bubbly Flow, Algebraic yPlus	bf	Yes	RANS-EVM	Algebraic yPlus	No
Bubbly Flow, L-VEL	bf	Yes	RANS-EVM	L-VEL	No
Bubbly Flow, k-ε	bf	Yes	RANS-EVM	k-ε	No
Bubbly Flow, Realizable k-ε	bf	Yes	RANS-EVM	Realizable k-ε	No
Bubbly Flow, k-ω	bf	Yes	RANS-EVM	k-ω	No
Bubbly Flow, SST	bf	Yes	RANS-EVM	SST	No
Bubbly Flow, Low Re k-ε	bf	Yes	RANS-EVM	Low Reynolds number k-ε	No
Bubbly Flow, Spalart–Allmaras	bf	Yes	RANS-EVM	Spalart–Allmaras	No
Bubbly Flow, v2-f	bf	Yes	RANS-EVM	v2-f	No

The **Bubbly Flow** ( ) branch interfaces are used primarily to model two-phase flow where the fluids are gas-liquid mixtures, and the gas content is less than 10%. The

Laminar Bubbly Flow Interface ( ) solves the Navier–Stokes equations with the momentum equation corrected by a term induced by the slip velocity. The slip velocity can be described by the Hadamard–Rybczynski drag law for small spherical bubbles, a nonlinear drag law taking surface tension into account for larger bubbles, or by defining it on your own.

The various forms of the Bubbly Flow, Turbulent Flow interfaces ( ) solve the RANS equations for the averaged velocity field and averaged pressure as well as models for the turbulent viscosity. The Bubbly Flow, Turbulent Flow interfaces include all the turbulence models available in the Single-Phase Flow, Turbulent Flow interfaces. See The Bubbly Flow Interfaces for links to the physics interface information.

By default, the physics interfaces assume that the volume fraction of the gas is less than 0.1. It is then valid to approximate the liquid velocity as incompressible. This is significantly easier to solve numerically. It is possible, though, to use the complete continuity equation.

The physics interfaces also allow you to define your own relations for the density of both phases and for the dynamic viscosity of the liquid phase. You can also model mass transfer between the two phases, using the two-film theory or your own expression for interfacial mass transfer.

MIXTURE MODEL INTERFACES

TABLE 6-2: MIXTURE MODEL DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	DISPERSED PHASE	SLIP MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL	SOLVE FOR INTERFACIAL AREA
Mixture Model, Laminar Flow	mm	Solid particles	Homogeneous flow	None	n/a	No
Mixture Model, Algebraic yPlus	mm	Solid particles	Homogeneous flow	RANS-EVM	Algebraic yPlus	No
Mixture Model, L-VEL	mm	Solid particles	Homogeneous flow	RANS-EVM	L-VEL	No
Mixture Model, k-ε	mm	Solid particles	Homogeneous flow	RANS-EVM	k-ε	No
Mixture Model, Realizable k-ε	mm	Solid particles	Homogeneous flow	RANS-EVM	Realizable k-ε	No
Mixture Model, k-ω	mm	Solid particles	Homogeneous flow	RANS-EVM	k-ω	No
Mixture Model, SST	mm	Solid particles	Homogeneous flow	RANS-EVM	SST	No

TABLE 6-2: MIXTURE MODEL DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	DISPERSED PHASE	SLIP MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL	SOLVE FOR INTERFACIAL AREA
Mixture Model, Low Re k-ε	mm	Solid particles	Homogeneous flow	RANS-EVM	Low Reynolds number k-ε	No
Mixture Model, Spalart–Allmaras	mm	Solid particles	Homogeneous flow	RANS-EVM	Spalart–Allmaras	No
Mixture Model, v2-f	mm	Solid particles	Homogeneous flow	RANS-EVM	v2-f	No

The **Mixture Model** ( ) branch interfaces are similar to the **Bubbly Flow** interfaces except that both phases are assumed to be incompressible. Examples include solid particles dispersed in a liquid, and liquid droplets dispersed in another liquid when the two liquids are immiscible.

Like the Bubbly Flow interfaces, The Mixture Model, Laminar Flow Interface ( ) and Mixture Model, Turbulent Flow interfaces ( ) solve the flow equations, whether described by the Navier–Stokes equations or the RANS equations with different turbulence models, and where the momentum equation is corrected by a term induced by the slip velocity. The slip velocity can be described by the Hadamard–Rybczynski, Schiller–Naumann or Haider–Levenspiel method, or by defining it on your own.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. The dynamic viscosity of the mixture can either be of Krieger type (which uses a maximum packing concentration), volume-averaged (for gas-liquid, liquid-liquid systems), or a user-defined expression.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature. The physics interfaces also allow you to model mass transfer between the two phases, using the two-film theory or your own expression for interfacial mass transfer.

EULER-EULER MODEL INTERFACES

TABLE 6-3: EULER-EULER MODEL DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	DISPERSED PHASE	DRAG MODEL	TURBULENCE MODEL TYPE
Euler-Euler Model, Laminar Flow	ee	Solid particles	Schiller–Naumann	None
Euler-Euler Model, Turbulent Flow	ee	Solid particles	Schiller–Naumann	RANS, k-ε

The **Euler-Euler Model** ( ) branch interfaces are used to model the flow of two continuous and fully interpenetrating phases. For both phases the conservation equations are averaged over volumes, which are small compared to the computational domain, but large compared to the dispersed phase particles, droplets, or bubbles. The Euler–Euler Model, Laminar Flow Interface solves two sets of conservation equations, one for each phase. The Euler–Euler Model, Turbulent Flow Interface additionally solves transport equations for the turbulence quantities, either using a mixture averaged turbulence models or solving separate transport equations for the turbulence quantities of each phase. The drag model for solid particles or liquid droplets/bubbles can be described by the Hadamard–Rybczynski, Schiller–Naumann or Ishii–Zuber, closures, or by defining it on your own. In addition the Haider–Levenspiel and Gidaspow closures are available for solid particles, and the Tomiyama and others closure is available for liquid droplets/bubbles.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. Predefined expressions for the dynamic viscosity of Krieger type (which uses a maximum packing concentration), are available.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature.

PHASE TRANSPORT MIXTURE MODEL INTERFACES

TABLE 6-4: PHASE TRANSPORT MIXTURE MODEL DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	DISPERSED PHASE	SLIP MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL
Phase Transport Mixture Model, Laminar Flow	Solid particles	Homogeneous flow	None	n/a
Phase Transport Mixture Model, Algebraic yPlus	Solid particles	Homogeneous flow	RANS-EVM	Algebraic yPlus
Phase Transport Mixture Model, L-VEL	Solid particles	Homogeneous flow	RANS-EVM	L-VEL
Phase Transport Mixture Model, k-ε	Solid particles	Homogeneous flow	RANS-EVM	k-ε
Phase Transport Mixture Model, Realizable k-ε	Solid particles	Homogeneous flow	RANS-EVM	Realizable k-ε
Phase Transport Mixture Model, k-ω	Solid particles	Homogeneous flow	RANS-EVM	k-ω
Phase Transport Mixture Model, SST	Solid particles	Homogeneous flow	RANS-EVM	SST
Phase Transport Mixture Model, Low Re k-ε	Solid particles	Homogeneous flow	RANS-EVM	Low Reynolds number k-ε
Phase Transport Mixture Model, Spalart–Allmaras	Solid particles	Homogeneous flow	RANS-EVM	Spalart–Allmaras
Phase Transport Mixture Model, v2-f	Solid particles	Homogeneous flow	RANS-EVM	v2-f

The **Phase Transport Mixture Model** ( ) branch interfaces are similar to the **Mixture Model** interfaces. The main difference is that the Phase Transport Mixture Model interfaces are multiphysics interfaces that couple a single-phase flow interface with a Phase Transport interface, allowing for multiple dispersed phases.

Like the Mixture Model interfaces, The Phase Transport Mixture Model, Laminar Flow and Turbulent Flow Interfaces solve the flow equations, whether described by the Navier–Stokes equations or the RANS equations with different turbulence models, and where the dispersed phase velocities are determined by the slip velocity. The slip velocity can be described by the Hadamard–Rybczynski, Schiller–Naumann or Haider–Levenspiel closures, or by defining it on your own.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. The dynamic viscosity of the mixture can either

be of Krieger type (which uses a maximum packing concentration), volume-averaged (for gas-liquid, liquid-liquid systems), or a user-defined expression.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature. The physics interfaces also enable you to model mass transfer between the two phases.

TABLE 6-5: TWO-PHASE FLOW, LEVEL SET DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-Phase Flow, Level Set	-	Two-phaseflow, level set	None	n/a	False
Two-Phase Flow, Level Set, Algebraic yPlus	-	Two-phaseflow, level set	RANS-EVM	Algebraic yPlus	False
Two-Phase Flow, Level Set, L-VEL	-	Two-phaseflow, level set	RANS-EVM	L-VEL	False
Two-Phase Flow, Level Set, k-ε	-	Two-phaseflow, level set	RANS-EVM	k-ε	False
Two-Phase Flow, Level Set, Realizable k-ε	-	Two-phaseflow, level set	RANS-EVM	Realizable k-ε	False
Two-Phase Flow, Level Set, k-ω	-	Two-phaseflow, level set	RANS-EVM	k-ω	False
Two-Phase Flow, Level Set, SST	-	Two-phaseflow, level set	RANS-EVM	SST	False
Two-Phase Flow, Level Set, Low Re k-ε	-	Two-phaseflow, level set	RANS-EVM	Low Reynolds number k-ε	False
Two-Phase Flow, Level Set, Spalart–Allmaras	-	Two-phaseflow, level set	RANS-EVM	Spalart–Allmaras	False
Two-Phase Flow, Level Set, v2f	-	Two-phaseflow, level set	RANS-EVM	v2f	False

TABLE 6-6: TWO-PHASE FLOW, PHASE-FIELD AND THREE-PHASE FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL TYPE	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-Phase Flow, Phase Field	-	Two-phaseflow, phase field	None	n/a	False
Two-Phase Flow, Phase Field, Algebraic yPlus	-	Two-phaseflow, phase field	RANS-EVM	Algebraic yPlus	False
Two-Phase Flow, Phase Field, L-VEL	-	Two-phaseflow, phase field	RANS-EVM	L-VEL	False
Two-Phase Flow, Phase Field, k-ε	-	Two-phaseflow, phase field	RANS-EVM	k-ε	False
Two-Phase Flow, Phase Field, Realizable k-ε	-	Two-phaseflow, phase field	RANS-EVM	Realizable k-ε	False
Two-Phase Flow, Phase Field, k-ω	-	Two-phaseflow, phase field	RANS-EVM	k-ω	False
Two-Phase Flow, Phase Field, SST	-	Two-phaseflow, phase field	RANS-EVM	SST	False
Two-Phase Flow, Phase Field, Low Re k-ε	-	Two-phaseflow, phase field	RANS-EVM	Low Reynolds number k-ε	False
Two-Phase Flow, Phase Field, Spalart–Allmaras	-	Two-phaseflow, phase field	RANS-EVM	Spalart–Allmaras	False
Two-Phase Flow, Phase Field, v2f	-	Two-phaseflow, phase field	RANS-EVM	v2f	False
Two-Phase Thin-Film Flow, Phase Field	-	Two-phase thin-film flow phase field	None	n/a	False
Laminar Three-Phase Flow, Phase Field	-	Three-phase flow, phase field	None	n/a	False

TABLE 6-7: TWO-PHASE FLOW, MOVING MESH PHYSICAL MODEL DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	COMPRESSIBILITY	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-Phase Flow, Moving Mesh	spf	not applicable	Incompressible flow	None

Two-Phase Flow, Level Set

The Laminar Two-Phase Flow, Level Set Interface ( ) and The Turbulent Two-Phase Flow, Level Set Interfaces ( ), found under the **Two-Phase Flow, Level Set** branch ( ), are used primarily to model two fluids separated by a fluid interface. The moving interface is tracked in detail using the level set method. Surface tension acting on the fluid interface can be included in the fluid-flow equations.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Level Set interface. The Stokes' flow option is available for low Reynolds number flows.

Specify the density for each of the two fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following non-Newtonian constitutive models are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou.

Two-Phase Flow, Phase Field

The Laminar Two-Phase Flow, Phase Field Interface ( ) and The Turbulent Two-Phase Flow, Phase Field Interfaces ( ) found under the **Two-Phase Flow, Phase Field** branch ( ), also model two fluids separated by a fluid interface. You can easily switch between the physics interfaces, which can be useful if you are not sure which physics interface provides the best description. Surface tension acting on the fluid interface are per default included in the fluid-flow equations. Library surface tension coefficients between a number of common substances are also available.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Phase Field interfaces. The Stokes' flow option is available for low Reynolds number flows.

Specify the density for each of the two fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following non-Newtonian constitutive models are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou.

Two-Phase Thin-Film Flow, Phase Field

The Two-Phase Thin-Film Flow, Domain, Phase Field Interface ( ), The Two-Phase Thin-Film Flow, Phase Field Interface for 2D ( ) and The Two-Phase Thin-Film Flow, Phase Field Interface for 3D ( ) found under the **Two-Phase Thin-Film Flow, Phase Field** branch ( ), model two fluids separated by a fluid interface, in a narrow channel represented by a domain, edge, or surface within the geometry. Surface tension acting on the fluid interface are per default included in the fluid-flow equations. Library surface tension coefficients between a number of common substances are also available.

Specify the density and viscosity for each of the two fluids. Density specification is not allowed when modified Reynolds equation option is chosen in the Thin-Film Flow interface.

Three-Phase Flow, Phase Field

The Laminar Three-Phase Flow, Phase Field Interface found under the **Three-Phase Flow, Phase Field** branch ( ) models flows of three incompressible fluids separated by sharp interfaces. Library surface tensions between a number of common substances are also available.

Specify the density for each of the three fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following non-Newtonian constitutive models are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou.

Two-Phase Flow, Moving Mesh

The Laminar Two-Phase Flow, Moving Mesh Interface , ( ) found under the **Multiphase Flow** > **Two-Phase Flow, Moving Mesh** branch ( ), is used primarily to model two fluids separated by a fluid interface. The moving interface is tracked as a boundary condition along a line or surface in the geometry. However, the method cannot accommodate topological changes in the boundary. Surface tension acting on the fluid interface are per default included in the fluid-flow equations. Library surface tension coefficients between a number of common substances are also available.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Moving Mesh interface. The Stokes' flow option is available for low Reynolds number flows.

Specify the density for each of the two fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following non-

Newtonian constitutive models are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou.

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple fluid flow to another type of phenomenon described in another physics interface. Although this is not often another type of flow, it can still involve physics interfaces supported in the CFD Module or in the COMSOL Multiphysics base package. This typically occurs in cases where applications include chemical reactions and mass transport, as included in Chemical Species Transport Interfaces, or energy transport, found in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of heat transfer, such as those involving radiation, can be found in the Heat Transfer Module, while tools for modeling chemical reactions and mass transport are available in the Chemical Reaction Engineering Module.

The Two-Phase Flow, Level Set and Phase Field Interfaces

The following sections list all the physics interfaces and the physics features associated with them under the **Multiphase Flow** branch ( ). The descriptions follow a structured order as defined by the order in the branch. Because many of the physics interfaces are integrated with each other, some nodes described also cross reference to other physics interfaces.

	Selecting the Right Physics Interface

This section includes the following topics:

- The Laminar Two-Phase Flow, Level Set Interface
- The Turbulent Two-Phase Flow, Level Set Interfaces
- The Two-Phase Flow, Level Set Coupling Feature
- The Wetted Wall Coupling Feature
- The Interior Wetted Wall Coupling Feature
- The Laminar Two-Phase Flow, Phase Field Interface
- The Turbulent Two-Phase Flow, Phase Field Interfaces
- The Two-Phase Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Laminar and Turbulent Flow, Two-Phase, Level Set and Phase Field Interfaces

	Mathematics, Moving Interface Branch

The Laminar Two-Phase Flow, Level Set Interface

The **Laminar Two-Phase Flow, Level Set** interface ( ) found under the **Multiphase Flow** > **Two-Phase Flow, Level Set** branch ( ), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that

is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Laminar Two-Phase Flow, Level Set** multiphysics interface, a **Laminar Flow** and a **Level Set** interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Level Set Coupling Feature, is added automatically under the **Multiphysics** node. The Wetted Wall Coupling Feature is also added, but with empty selection. Other **Wetted Wall** multiphysics coupling features and The Interior Wetted Wall Coupling Feature can be added when needed to model walls.

Simulations using the Laminar Two-Phase Flow, Level Set interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Turbulence Model

By default the **Turbulence model type** selected is **None**.

Discretization

By default the fluid flow discretization is set to **P1+P1**, and the level set discretization is set to **Linear**. This combination provides exact conservation of the integral of the level set variable when using the nonconservative form of the level set equation.

- Theory for the Two-Phase Flow Interfaces
- Theory for the Single-Phase Flow Interfaces

The Turbulent Two-Phase Flow, Level Set Interfaces

The **Turbulent Two-Phase Flow, Level Set** interfaces ( ) found under the **Multiphase Flow** > **Two-Phase Flow, Level Set** branch ( ), are multiphysics interfaces designed to track the interface between two immiscible fluids. The flow is assumed to be turbulent, that is, to be of high Reynolds number. The fluids can be incompressible or compressible.

When adding a **Turbulent Two-Phase Flow, Level Set** multiphysics interface, a **Turbulent Flow** interface and a **Level Set** interface are added in the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Level Set Coupling Feature, is

automatically added under the **Multiphysics** node. Another multiphysics coupling feature, The Wetted Wall Coupling Feature, can be added when needed.

- The **Turbulent Flow, Algebraic yPlus** interface ( ) combines a Level Set interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface ( ) combines a Level Set interface with a Turbulent Flow, L-VEL interface.
- The **Turbulent Flow, k-ε** interface ( ) combines a Level Set interface with a Turbulent Flow, k-ε interface.
- The **Turbulent Flow, Realizable k-ε** interface ( ) combines a Level Set interface with a Turbulent Flow, Realizable k-ε interface.
- The **Turbulent Flow, k-ω** interface ( ) combines a Level Set interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, SST** interface ( ) combines a Level Set interface with a Turbulent Flow, SST interface.
- The **Turbulent Flow, Low Re k-ε** interface ( ) combines a Level Set interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, Spalart–Allmaras** interface ( ) combines a Level Set interface with a Turbulent Flow, Spalart–Allmaras interface.
- The **Turbulent Flow, v2-f** interface ( ) combines a Level Set interface with a Turbulent Flow, v2-f interface.

Simulations using the Turbulent Two-Phase Flow, Level Set interfaces are always time-dependent since the position of an interface almost always depends on its history.

INTERFACE PROPERTIES

Turbulence Model

By default the **Turbulence model type** selected is **RANS-EVM**. Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM**.

- Theory for the Two-Phase Flow Interfaces
- Theory for the Single-Phase Flow Interfaces

The Two-Phase Flow, Level Set Coupling Feature

The **Laminar Two-Phase Flow, Level Set** ( ) and **Turbulent Two-Phase Flow, Level Set** () interfaces contain a multiphysics coupling feature, **Two-Phase Flow, Level Set**, which is added automatically.

The **Two-Phase Flow, Level Set** multiphysics coupling feature defines the density and dynamic viscosity of the fluid used in the **Laminar Flow** or **Turbulent Flow** interface, and it defines the surface tension on the interface in form of a volume force used in the momentum equation. It also enables the **Level Set** interface to use the velocity field calculated from the **Laminar Flow** or **Turbulent Flow** interface to transport the interface.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Level Set** in the model) is `tpf1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

MODEL INPUTS

Fluid properties of each phase, such as density, viscosity, or the surface tension coefficient, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p + p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIAL PROPERTIES

The effective density and dynamic viscosity can either be **Locally defined** or picked up from a Multiphase Material. When the properties are defined locally, provide the properties for each phase in the respective fluid properties section, and the averaging method in the advanced settings section. If a multiphase material is used, these settings are controlled from the material. Using a multiphase material is advantageous for models coupling two-phase flow with other physics interfaces, such as Heat Transfer in Fluids or Electrostatics. In such cases, the multiphase material can ensure that the effective material properties for these physics interfaces are averaged using the volume fraction from the Level Set physics interface.

Click the **Go to Material** button ( ) to move to the selected material node. Click the **Add Multiphase Material** button ( ) to add a multiphase material with two phases. The added material then becomes the one selected in the **Multiphase Material** list.

Multiphase Material in the *COMSOL Multiphysics Reference Manual*

FLUID PROPERTIES

A **Fluid Properties** section will be available per phase if the **Material Properties** are set to **Locally defined**. Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid 1** from a material, select the appropriate material in the **Fluid 1** list. Also make sure that the **Density of fluid 1** ρ_1 and **Dynamic viscosity of fluid 1** μ_1 are both set to **From Material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the fluid flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models can alternatively be used to specify the dynamic viscosities of the two fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid 1** ρ_1 or the **Dynamic viscosity of fluid 1** μ_1 list and enter the expression in the corresponding text field.

Similarly, the properties of **Fluid 2** can be specified. The default material is set to **None**.

Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2. The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason, selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

ADVANCED SETTINGS

If the **Material Properties** are set to **Locally defined**, you can specify the averaging method for density and dynamic viscosity in this section. The default method for **Density averaging** and **Viscosity averaging** is **Volume average**. In addition to the default method, **Density averaging** can be set to **Heaviside function** or **Harmonic volume average**, while **Viscosity averaging** can be set to **Heaviside function**, **Harmonic volume average**, **Mass average**, or **Harmonic mass average**. When a **Heaviside function** is used, enter a value for the corresponding mixing parameter, l_ρ or l_μ.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation. The surface tension force is not added to porous domains.

Select a **Surface tension coefficient** σ (SI unit: N/m):

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air** or **Glycerol/Air**). The predefined correlations are based on the data in Ref. 7, Ref. 8, and Ref. 9.
- For **User defined** enter a value or expression for the surface tension coefficient σ (SI unit: N/m).

The Wetted Wall Coupling Feature

The **Laminar Two-Phase Flow, Level Set** ( ) and **Turbulent Two-Phase Flow, Level Set** ( ) interfaces contain an optional multiphysics coupling boundary feature, **Wetted Wall**. It is an exclusive feature that overrides the **Wall** feature in the Laminar or Turbulent Flow interface as well as the **No Flow** feature in the Level Set interface. It cannot be used in boundaries that have a **Flow Continuity** feature in the flow physics interface or a **Continuity** feature in the level set physics interface. It is available for laminar flow and turbulent flow with wall functions or automatic wall treatment.

The **Wetted Wall** boundary condition is suitable for walls in contact with the fluid-fluid interface. When this boundary condition is used, the fluid-fluid interface can move along the wall.

For laminar flow, this boundary condition enforces the no-penetration condition $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$ and adds a tangential stress on the form

$$\mathbf{K}_{\text{nt}} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\mathbf{K}_{\text{nt}} = \mathbf{K}_{\text{n}} - (\mathbf{K}_{\text{n}} \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$, $\mathbf{K}_{\text{n}} = \mathbf{K}\mathbf{n}_{\text{wall}}$, and $\mathbf{K}$ is the viscous stress tensor. β is the slip length. For numerical calculations, a suitable choice is $\beta = h$, where h is the mesh element size. The boundary condition does not set the tangential velocity component to zero. However, the extrapolated tangential velocity component is 0 at a distance β outside the wall (see Figure 6-1).

For turbulent flow, the wall is modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the turbulent flow interface settings.

If the surface tension force is included in the momentum equation in The Two-Phase Flow, Level Set Coupling Feature, the **Wetted Wall** boundary condition also adds the following boundary force to enforce the contact angle:

$$\mathbf{F}_{\theta} = \sigma\delta(\mathbf{n}_{\text{wall}} \cdot \mathbf{n} - \cos\theta_{\text{w}})\mathbf{n}$$

The contact angle θ_{w} is defined as the angle between the fluid interface and the wall (see Figure 6-1). For more information, see Ref. 4 and Ref. 5. Note that the contact angle is not enforced on boundaries adjacent to porous domains.

The contact angle θ_{w} can be defined directly or from Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_w) + \gamma_{s2} = \gamma_{s1} \tag{6-1}$$

where γ_{s1} is the surface energy density on the fluid 1 — solid (wall) interface and γ_{s2} is the surface energy density on the fluid 2 — solid (wall) interface.

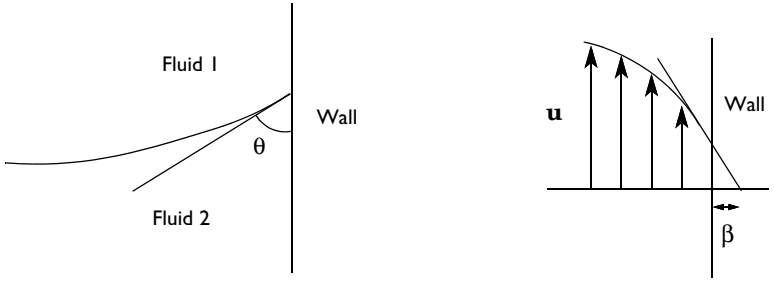

Figure 6-1: Definition of the contact angle θ *at interface/wall contact points (left) and an illustration of the slip length* β *(right).*

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Wetted Wall** multiphysics coupling feature in the model) is `ww1`.

BOUNDARY SELECTION

When nodes are added from the context menu, select **All boundaries** (the default) or select **Manual** from the **Selection** list to choose specific boundaries.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{tr}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model

component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame. For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the φ-component of $\mathbf{u_{tr}}$ can also be specified.

Translational velocity can also be set to **Zero (Fixed wall)** to force $\mathbf{u_{tr}} = \mathbf{0}$. This is typically used in problems where the mesh is deforming or rotating, but we want the boundary to keep zero velocity. For example, in fixed walls tangential to a **Rotating Domain**.

WETTED WALL

When using **Navier Slip**, the **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input. Select **User defined** from **Slip Length** selection list in order to manually prescribe β (SI unit: m).

If the fluid physics interface includes porous domains, check **Use porous slip wall treatment** to use the porous slip wall treatment to provide tangential stresses and the slip velocity on boundaries adjacent to porous domains. If **Use porous slip wall treatment** is not checked, the condition selected in **Wall condition** is used for porous boundaries.

CONTACT ANGLE

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**. For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians. For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

Theory for the Two-Phase Flow Interfaces

The Interior Wetted Wall Coupling Feature

The **Interior Wetted Wall**, multiphysics coupling boundary feature can only be applied on interior boundaries.

It is similar to The Wetted Wall Coupling Feature available on exterior boundaries of the **Laminar Two-Phase Flow, Level Set** ( ) and **Turbulent Two-Phase Flow, Level Set** ( ) multiphysics interfaces, except that it applies on both sides of an interior boundary. It is an exclusive feature which overrides the **Interior Wall** feature in the Laminar or Turbulent Flow interface as well as the **Thin Barrier** feature in the Level Set interface. It is available for laminar flow and turbulent flow with wall functions or automatic wall treatment.

The **Interior Wetted Wall** coupling feature allows discontinuities (velocity, pressure, level set variable, and turbulence variables) across the boundary and can be used to avoid meshing thin structures in contact with the fluid-fluid interface. When this boundary condition is used, the fluid-fluid interface can move along the wall.

For laminar flow, this boundary condition enforces the no-penetration condition $\mathbf{u} \cdot \mathbf{n}_{\text{wall}} = 0$ on both sides of the wall, and adds a tangential stress on the form

$$\mathbf{K}_{\text{nt}} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\mathbf{K}_{\text{nt}} = \mathbf{K}_{\text{n}} - (\mathbf{K}_{\text{n}} \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$, $\mathbf{K}_{\text{n}} = \mathbf{K}\mathbf{n}_{\text{wall}}$, and $\mathbf{K}$ is the viscous stress tensor. β is the slip length. For numerical calculations, a suitable choice is $\beta = h$, where h is the mesh element size.

For turbulent flow, the wall is modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the turbulent flow interface settings.

If the surface tension force is included in the momentum equation, the **Interior Wetted Wall** boundary condition also adds the following boundary force on both sides of the walls to enforce the contact angle:

$$\mathbf{F}_{\theta} = \sigma\delta(\mathbf{n}_{\text{wall}} \cdot \mathbf{n} - \cos\theta_{\text{w}})\mathbf{n}$$

Note that the contact angle is not enforced on boundaries adjacent to porous domains. For more information, see The Wetted Wall Coupling Feature.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Interior Wetted Wall** multiphysics coupling feature in the model) is `iww1`.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame. For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the φ-component of $\mathbf{u_{tr}}$ can also be specified.

BOUNDARY SELECTION

When nodes are added from the context menu, select **All boundaries** (the default) or select **Manual** from the **Selection** list to choose specific boundaries.

WETTED WALL

When using **Navier Slip**, the **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input. Select **User defined** from **Slip Length** selection list in order to manually prescribe β (SI unit: m).

If the fluid physics interface includes porous domains, check **Use porous slip wall treatment** to use the porous slip wall treatment to provide tangential stresses and the slip velocity on boundaries adjacent to porous domains. If **Use porous slip wall treatment** is not checked, the condition selected in **Wall condition** is used for porous boundaries.

CONTACT ANGLE

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**. For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians. For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

The Wetted Wall Coupling Feature

The Laminar Two-Phase Flow, Phase Field Interface

The **Laminar Two-Phase Flow, Phase Field** interface ( ) found under the **Multiphase Flow** > **Two-Phase Flow, Phase Field** branch ( ), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the **Laminar Two-Phase Flow, Phase Field** multiphysics interface, a **Laminar Flow** and a **Phase Field in Fluids** interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Phase Field Coupling Feature, is added automatically under the **Multiphysics** node. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall feature here is not implemented as a separate multiphase coupling boundary feature but as a default **Wetted Wall** feature in the **Phase Field in Fluids** interface.

Wetted Wall

Simulations using the Laminar Two-Phase Flow, Phase Field interface are always time-dependent since the position of an interface almost always depends on its history.

INTERFACE PROPERTIES

Turbulence Model

By default the **Turbulence model type** selected is **None**. Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM**.

Discretization

By default the fluid flow discretization is set to **P1+P1**, and the phase field discretization is set to **Linear**. This combination provides improved conservation of the integral of the phase field variable when using the nonconservative form of the phase field equations.

Theory for the Two-Phase Flow Interfaces

The Turbulent Two-Phase Flow, Phase Field Interfaces

The **Turbulent Two-Phase Flow, Phase Field** interfaces ( ) found under the **Multiphase Flow** > **Two-Phase Flow, Phase Field** branch ( ), are multiphysics interfaces designed to track the interface between two immiscible fluids. The flow is by default assumed to be turbulent. The fluids can be incompressible or compressible.

When adding a **Turbulent Two-Phase Flow, Phase Field** multiphysics interface, a **Turbulent Flow** and a **Phase Field in Fluids** interface are added in the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Phase Field Coupling Feature, is automatically added under the **Multiphysics** node. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall feature here is not implemented as a separate multiphase coupling boundary feature but as a default feature in the **Phase Field in Fluids** interface.

Wetted Wall

- The **Turbulent Flow, Algebraic yPlus** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, L-VEL interface.
- The **Turbulent Flow, k-ε** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, k-ε interface.

- The **Turbulent Flow, Realizable k-ε** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, Realizable k-ε interface
- The **Turbulent Flow, k-ω** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, SST** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, SST interface.
- The **Turbulent Flow, Low Re k-ε** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, Spalart–Allmaras** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, Spalart–Allmaras interface.
- The **Turbulent Flow, v2-f** interface ( ) combines a Phase Field in Fluids interface with a Turbulent Flow, v2-f interface.

Simulations using the Turbulent Two-Phase Flow, Phase Field interfaces are always time-dependent since the position of an interface almost always depends on its history.

INTERFACE PROPERTIES

Turbulence Model

By default the **Turbulence model type** selected is **RANS-EVM**. If **None** is selected for **Turbulence model type**, the model becomes laminar.

Theory for the Two-Phase Flow Interfaces

The Two-Phase Flow, Phase Field Coupling Feature

The **Laminar Two-Phase Flow, Phase Field** ( ) and **Turbulent Two-Phase Flow, Phase Field** ( ) interfaces contain a multiphysics coupling feature, **Two-Phase Flow, Phase Field**, which is added automatically.

The **Two-Phase Flow, Phase Field** multiphysics coupling feature defines the density and dynamic viscosity of the fluid used in the **Laminar Flow** and **Turbulent Flow** interfaces, and it defines the surface tension on the interface in form of a volume force used in the momentum equation. It also enables the **Phase Field in Fluids** interface to use the velocity field calculated from the **Laminar Flow** or **Turbulent Flow** interface to transport the interface.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Phase Field** in the model) is `tpf1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

MODEL INPUTS

Fluid properties of each phase, such as density, viscosity, or the surface tension coefficient, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p+p_{\mathrm{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIAL PROPERTIES

The effective density and dynamic viscosity can either be **Locally defined** or picked up from a Multiphase Material. When the properties are defined locally, provide the properties for each phase in the respective fluid properties section, and the averaging method in the advanced settings section. If a multiphase material is used, these settings are controlled from the material. Using a multiphase material is advantageous for models coupling two-phase flow with other physics interfaces, such as Heat Transfer in Fluids or Electrostatics. In such cases, the multiphase material can ensure that the effective material properties for these physics interfaces are averaged using the volume fraction from the Phase Field in Fluids physics interface.

Click the **Go to Material** button ( ) to move to the selected material node. Click the **Add Multiphase Material** button ( ) to add a multiphase material with two phases. The added material then becomes the one selected in the **Multiphase Material** list.

Multiphase Material in the *COMSOL Multiphysics Reference Manual*

- *Separation Through Electrocoalescence*: Application Library path **CFD_Module/Multiphase_Flow/electrocoalescence**

FLUID PROPERTIES

A **Fluid Properties** section will be available per phase if the **Material Properties** are set to **Locally defined**. Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid 1** from a material, select the appropriate material in the **Fluid 1** list. Also make sure that the **Density of fluid 1** ρ_1 and **Dynamic viscosity of fluid 1** μ_1 are both set to **From Material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the fluid flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models can alternatively be used to specify the dynamic viscosities of the two fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid 1** ρ_1 or the **Dynamic viscosity of fluid 1** μ_1 list and enter the expression in the corresponding text field.

Similarly, the properties of **Fluid 2** can be specified. The default material is set to **None**.

Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2. The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason, selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

The fluid defined as Fluid 1 affects the wetting characteristics on wetted walls. See the Wetted Wall node for details.

ADVANCED SETTINGS

f the **Material Properties** are set to **Locally defined**, you can specify the averaging method for density and dynamic viscosity in this section. Select the method used for **Density averaging** and **Viscosity averaging**. The default method for both settings is **Volume average**. In addition to the default method, **Density averaging** can be set to **Heaviside function** or **Harmonic volume average**, while **Viscosity averaging** can be set to **Heaviside function**, **Harmonic volume average**, **Mass average**, or **Harmonic mass average**. When a

Heaviside function is used, enter a value for the corresponding mixing parameter, l_ρ or l_μ.

When the surface tension force is included in the momentum equation, you can select the **Shift surface tension force to the heaviest phase** checkbox. This can prevent significant spurious oscillations in the velocity field for the lighter phase in cases with a large difference in density between the two phases. The amount of shifting is controlled by the **Smoothing factor** $d_{s,Fst}$ (default 0.1). The surface tension force is then multiplied by

$$f_s = \frac{2}{(\rho_1 + \rho_2)}\left(\rho_1 H\left(\frac{V_{f,1} - 0{,}5}{d_{s,Fst}}\right) + \rho_2 H\left(\frac{V_{f,2} - 0{,}5}{d_{s,Fst}}\right)\right) \quad (6\text{-}2)$$

Shift surface tension force to the heaviest phase works better when combined with **Heaviside function** for the averaging of density and viscosity.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation. If the surface tension force is included, select **Include surface tension gradient effects in surface tension force** to account for the Marangoni effect due to gradients in the surface tension coefficient.

Select a **Surface tension coefficient** σ (SI unit: N/m):

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air** or **Glycerol/Air**). The predefined correlations are based on the data in Ref. 7, Ref. 8, and Ref. 9.
- For **User defined**, enter a value or expression for the surface tension coefficient σ (SI unit: N/m).

Theory for the Two-Phase Flow Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar and Turbulent Flow, Two-Phase, Level Set and Phase Field Interfaces

The Two-Phase Flow, Level Set and Phase Field interfaces are multiphysics interfaces combining Laminar Flow or Turbulent Flow interfaces together with Level Set or Phase Field in Fluids interfaces.

LAMINAR FLOW

The available physics features for the Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW

The available physics features for the Turbulent Flow interface are also listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LEVEL SET

The available physics features for the Level Set interface are listed in the section Domain, Boundary, and Pair Nodes for the Level Set Interface.

PHASE FIELD IN FLUIDS

The available physics features for the Phase Field in Fluids interface are listed in the section Domain, Boundary, and Pair Nodes for the Phase Field in Fluids Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Two-Phase Thin-Film Flow, Phase Field Interfaces

The following sections list all the physics interfaces and the physics features associated with the Two-Phase Thin-Film Flow, Phase Field interfaces, located under the **Multiphase Flow** branch ( ).

	Selecting the Right Physics Interface

This section includes the following topics:

- The Two-Phase Thin-Film Flow, Domain, Phase Field Interface
- The Two-Phase Thin-Film Flow, Phase Field Interface for 2D
- The Two-Phase Thin-Film Flow, Phase Field Interface for 3D
- The Two-Phase Thin-Film Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Two-Phase Thin-Film Flow, Phase Field Interfaces

	Mathematics, Moving Interface Branch

The Two-Phase Thin-Film Flow, Domain, Phase Field Interface

The **Two-Phase Thin-Film Flow, Domain, Phase Field** interface ( ) found under the **Multiphase Flow** > **Two-Phase Thin-Film Flow, Phase Field** branch ( ), is a multiphysics interface designed to track the interface between two immiscible fluids. The fluids are assumed to flow in a narrow channel that is represented by a domain within the geometry.

When adding the **Two-Phase Thin-Film Flow, Domain, Phase Field** multiphysics interface, a **Thin-Film Flow, Domain** and a **Phase Field Thin-Film Flow** interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Thin-Film Flow, Phase Field Coupling Feature, is added automatically under the **Multiphysics** node.

Simulations using the **Two-Phase Thin-Film Flow, Domain, Phase Field** interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Discretization

By default the fluid flow discretization is set to **P1+P1**, and the phase field discretization is set to **Linear**. This combination provides an improved conservation of the integral of the phase field variable when using the nonconservative form of the phase field thin-film flow equations.

- Theory for the Two-Phase Thin-Film Flow, Phase Field Interfaces

The Two-Phase Thin-Film Flow, Phase Field Interface for 2D

The **Two-Phase Thin-Film Flow, Phase Field** interface ( ) found under the **Multiphase Flow** > **Two-Phase Thin-Film Flow, Phase Field** branch ( ), is a multiphysics interface designed to track the interface between two immiscible fluids. The fluids are assumed to flow in a narrow channel that is represented by an edge within the geometry.

When adding the **Two-Phase Thin-Film Flow, Phase Field** multiphysics interface, a **Thin-Film Flow** and a **Phase Field Thin-Film Flow** interfaces are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Thin-Film Flow, Phase Field Coupling Feature, is added automatically under the **Multiphysics** node.

Simulations using the **Two-Phase Thin-Film Flow, Phase Field** interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Discretization

By default the fluid flow discretization is set to **P1+P1**, and the phase field discretization is set to **Linear**. This combination provides an improved conservation of the integral of

the phase field variable when using the nonconservative form of the phase field thin-film flow equation.

- Theory for the Two-Phase Thin-Film Flow, Phase Field Interfaces

The Two-Phase Thin-Film Flow, Phase Field Interface for 3D

The **Two-Phase Thin-Film Flow, Phase Field** interface ( ) found under the **Multiphase Flow** > **Two-Phase Thin-Film Flow, Phase Field** branch ( ), is a multiphysics interface designed to track the interface between two immiscible fluids. The fluids are assumed to flow in a narrow channel that is represented by a surface within the geometry.

When adding the **Two-Phase Thin-Film Flow, Phase Field** multiphysics interface, a **Thin-Film Flow** and a **Phase Field Thin-Film Flow** interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Thin-Film Flow, Phase Field Coupling Feature, is added automatically under the **Multiphysics** node.

Simulations using the **Two-Phase Thin-Film Flow, Phase Field** interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Discretization

By default the fluid flow discretization is set to **P1+P1**, and the phase field discretization is set to **Linear**. This combination provides an improved conservation of the integral of the phase field variable when using the nonconservative form of the phase field thin-film flow equations.

- Theory for the Two-Phase Thin-Film Flow, Phase Field Interfaces

The Two-Phase Thin-Film Flow, Phase Field Coupling Feature

The **Two-Phase Thin-Film Flow, Phase Field** ( ) interface contains a multiphysics coupling feature, **Two-Phase Thin-Film Flow, Phase Field**, which is added automatically.

The **Two-Phase Thin-Film Flow, Phase Field** multiphysics coupling feature defines the density and dynamic viscosity of the fluid used in the **Thin-Film Flow** interface, and it

defines the surface tension on the interface in form of a volume force used in the momentum equation. It also enables the **Phase Field** interface or the **Phase Field Thin-Film Flow** interface to use the velocity field calculated from the **Thin-Film Flow** interface to transport the interface.

The multiphysics coupling is not available for boundaries (edges in 2D problems) with **Cavitation** option enabled in the **Thin-Film Flow** interface.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Thin-Film Flow, Phase Field** in the model) is `tpf1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

MODEL INPUTS

Fluid properties of each phase, such as density, viscosity, or the surface tension coefficient, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field

can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIAL PROPERTIES

The effective density and dynamic viscosity can either be **Locally defined** or picked up from a Multiphase Material. When the properties are defined locally, provide the properties for each phase in the respective fluid properties section, and the averaging method in the advanced settings section. If a multiphase material is used, these settings are controlled from the material. Using a multiphase material is advantageous for models coupling two-phase flow with other physics interfaces, such as Heat Transfer in Fluids or Electrostatics. In such cases, the multiphase material can ensure that the effective material properties for these physics interfaces are averaged using the volume fraction from the Level Set physics interface.

Click the **Go to Material** button ( ) to move to the selected material node. Click the **Add Multiphase Material** button ( ) to add a multiphase material with two phases. The added material then becomes the one selected in the **Multiphase Material** list.

Multiphase Material in the *COMSOL Multiphysics Reference Manual*

FLUID PROPERTIES

A **Fluid Properties** section will be available per phase if the **Material Properties** are set to **Locally defined**. Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid 1** from a material, select the appropriate material in the **Fluid 1** list. Also make sure that the **Density of fluid 1**, ρ_1, and **Dynamic viscosity of fluid 1**, μ_1, are both set to **From Material**.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid 1**, ρ_1 or the **Dynamic viscosity of fluid 1**, μ_1 list and enter the expression in the corresponding text field.

Similarly, the properties of **Fluid 2** can be specified. The default material is set to **None**.

The specification of densities for the two fluids is not available when the Modified Reynolds Equation option is chosen in the **Thin-Film Flow** interface.

Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2. The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason, selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

ADVANCED SETTINGS

If the **Material Properties** are set to **Locally defined**, you can specify the averaging method for density and dynamic viscosity in this section. The default method for **Density averaging** and **Viscosity averaging** is **Volume average**. In addition to the default method, **Density averaging** can be set to **Heaviside function** or **Harmonic volume average**, while **Viscosity averaging** can be set to **Heaviside function**, **Harmonic volume average**, **Mass average**, or **Harmonic mass average**. When a **Heaviside function** is used, enter a value for the corresponding mixing parameter, l_ρ or l_μ.

The specification of the **Density averaging** is not available when the Modified Reynolds Equation option is chosen in the **Thin-Film Flow** interface.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation. Select a **Surface tension coefficient** σ (SI unit: N/m):

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air** or **Glycerol/Air**).
- For **User defined**, enter a value or expression for the surface tension coefficient σ (SI unit: N/m).

Theory for the Two-Phase Thin-Film Flow, Phase Field Interfaces

Domain, Boundary, Point, and Pair Nodes for the Two-Phase Thin-Film Flow, Phase Field Interfaces

The Two-Phase Thin-Film Flow, Phase Field interfaces are multiphysics interfaces combining Thin-Film Flow interfaces together with Phase Field interfaces or the Phase Field Thin-Film Flow interfaces.

THIN-FILM FLOW

The available physics features for the Thin-Film Flow interfaces are listed in the section Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Interfaces.

PHASE FIELD IN FLUIDS

The available physics features for the Phase Field in Fluids are listed in the section Domain, Boundary, and Pair Nodes for the Phase Field in Fluids Interface.

PHASE FIELD THIN-FILM FLOW

The available physics features for the Phase Field Thin-Film Flow interfaces are listed in the section Boundary, Edge, and Point Nodes for the Phase Field Thin-Film Flow Interfaces.

All domain, boundary, edge, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Three-Phase Flow, Phase Field Interface

This section includes the following topics:

- The Laminar Three-Phase Flow, Phase Field Interface
- The Three-Phase Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

	Mathematics, Moving Interface Branch

The Laminar Three-Phase Flow, Phase Field Interface

The **Laminar Three-Phase Flow, Phase Field** interface (), found under the **Multiphase Flow** > **Three-Phase Flow, Phase Field** branch (), is a multiphysics interface designed to track the interfaces between three immiscible and incompressible fluids. The flow is assumed to be laminar; that is, a flow characterized by a low-to-moderate Reynolds number. The density of each fluid is assumed to be constant, but the there is no restriction on the density differences between the separate fluids.

When adding the **Laminar Three-Phase Flow, Phase Field** multiphysics interface, a **Laminar Flow** and a **Ternary Phase Field** interface are added to the Model Builder. In addition the **Multiphysics** node, including the multiphysics coupling feature **Three-Phase Flow, Phase Field** is added.

	The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

Simulations using the Laminar Three-Phase Flow, Phase Field interface are always time-dependent since the position of an interface almost always depends on its history.

The Three-Phase Flow, Phase Field Coupling Feature

Use the **Three-Phase Flow, Phase Field** ( ) multiphysics coupling to simulate the flow of a three immiscible fluids while explicitly tracking the interface separating each pair of the fluids.

The Three-Phase Flow interface solves Navier–Stokes equations for the conservation of momentum, and a continuity equation for the conservation of mass. The positions of the interfaces separating the fluid phases are tracked by solving four additional transport equations: two equations governing phase field variables and two equations for the corresponding generalized chemical potentials. The movement of the fluid-fluid interfaces is determined by minimization of free energy.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `tfpf1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the three-phase flow, or select **All domains** as needed.

MODEL INPUTS

Fluid properties of each phase, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own

tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p + p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIAL PROPERTIES

The effective density and dynamic viscosity can either be **Locally defined** or picked up from a Multiphase Material. When the properties are defined locally, provide the properties for each phase in the respective fluid properties section, and the averaging method in the advanced settings section. If a multiphase material is used, these settings are controlled from the material. Using a multiphase material is advantageous for models coupling two-phase flow with other physics interfaces, such as Heat Transfer in Fluids or Electrostatics. In such cases, the multiphase material can ensure that the effective material properties for these physics interfaces are averaged using the volume fraction from the Ternary Phase Field physics interface.

Click the **Go to Material** button ( ) to move to the selected material node. Click the **Add Multiphase Material** button ( ) to add a multiphase material with three phases. The added material then becomes the one selected in the **Multiphase Material** list.

Multiphase Material in the *COMSOL Multiphysics Reference Manual*

FLUID PROPERTIES

A **Fluid Properties** section will be available per phase if the **Material Properties** are set to **Locally defined**. Use the corresponding section to specify the properties of all three fluids. The fluids are denoted **Fluid A**, **Fluid B**, and **Fluid C**, respectively.

To specify the properties of **Fluid A** from a material, select the appropriate material in the **Fluid A** list. Also make sure that the **Density of fluid A** ρ_A and **Dynamic viscosity of fluid A** μ_A are both set to **From material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the laminar flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley–Papanastasiou, and Casson–Papanastasiou models can alternatively be used to specify the dynamic viscosities of the three fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid A** ρ_A or the **Dynamic viscosity of fluid A** μ_A list and enter the expression in the corresponding text field.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

- Theory for the Two-Phase Flow Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

The Two-Phase Thin-Film Flow, Phase Field Interfaces is a multiphysics interface combining The Laminar Flow Interface and The Phase Field Thin-Film Flow Interfaces.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TERNARY PHASE-FIELD

The available physics features for The Phase Field Thin-Film Flow Interfaces are listed in Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Laminar Two-Phase Flow, Moving Mesh Interface

The **Laminar Two-Phase Flow, Moving Mesh** interface ( ), found under the **Multiphase Flow** > **Two-Phase Flow, Moving Mesh** branch ( ), is a multiphysics interface designed to model laminar two–phase flow of immiscible fluids separated by a moving interface. The velocity field, pressure, and mesh deformation are solved for, and the location of the interface is tracked by the deformed mesh.

When adding the **Laminar Two-Phase Flow, Moving Mesh** multiphysics interface, a **Laminar Flow** interface is added to the component, and a **Moving Mesh** interface with a **Deforming Domain** feature is added under the **Definitions** node. The **Laminar Flow** interface adds the Navier–Stokes equations and provides a way of defining the properties of the fluids. For each of the fluids the density and viscosity must be specified (these are typically taken from the corresponding materials, but can be user defined).

Simulations using the **Laminar Two-Phase Flow, Moving Mesh** interface are always time-dependent since the position of an interface is almost always dependent of its history. There are additional boundary conditions to describe how the fluid-fluid interface moves from the **Laminar Flow** context menu under the option **Fluid Interface Features**:

- Fluid-Fluid Interface
- Free Surface
- Contact Angle (as a subfeature to the two conditions above)

In previous versions of COMSOL Multiphysics (prior to version 5.4), a specific physics interface called **Laminar Two-Phase Flow, Moving Mesh (tpfmm)** was added to the **Model Builder**. Now, a predefined multiphysics coupling approach is used, improving the flexibility and design options for your modeling. For specific details, see The Multiphysics Branch and Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

Select Laminar Flow Properties

For a full list of available properties, see The Laminar Flow Interface.

PHYSICAL MODEL

This physics interface deforms the mesh within the domains on either side of the two fluid interfaces to track its movement.

The **Compressibility** defaults to **Incompressible flow** to use the incompressible (constant density) formulation of the Navier–Stokes equations. Select **Compressible flow (Ma<0.3)** to use the compressible formulation.

If flow is occurring at very low Reynolds numbers, the inertial term in the Navier–Stokes equations can be neglected and the linear Stokes equations can be solved on the domain. This flow type is referred to as *creeping flow* or *Stokes flow* and can occur in microfluidics and MEMS devices, where the flow length scales are very small. To make this approximation select the **Neglect inertial term (Stokes flow)** checkbox, which significantly improves the solver speed.

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

DEPENDENT VARIABLES

The dependent variables (field variables) are for the **Velocity field** and **Pressure**. The names can be changed in the corresponding fields, but the names of fields and dependent variables must be unique within a model.

The following models are found at this Application Library path **CFD_Module/Multiphase_Flow/<filename>**

- *Drug Delivery System*: **viscous_catenary**
- *Electrowetting Lens*: **electrowetting_lens**
- *Viscous Catenary*: **viscous_catenary**

Deforming Domain

When the **Laminar Two-Phase Flow, Moving Mesh** multiphysics interface is added using the **Model Wizard**, a **Deforming Domain** node is added automatically in the **Model Builder** under the **Definitions** > **Moving Mesh** node. This node serves to represent domains and boundaries where the mesh can deform. By default, the selection is all domains. Under the **Deforming Domain**, you can also choose the **Mesh smoothing type**, by default set to

Yeoh with a default **Stiffening factor** of 10. More information of the smoothing type can be found in the Deforming Domain chapter in the *COMSOL Multiphysics Reference Manual*.

By default, the mesh is fixed at all external boundaries of the geometry. Use the Symmetry/Roller node to select the external boundaries, where the fluid-fluid interface can slide along the boundary. You can also add other types of boundary conditions for the mesh motion, for details see Moving Mesh Features in the *COMSOL Multiphysics Reference Manual*.

Fluid-Fluid Interface

The **Fluid-Fluid Interface** node defines the initial position of a fluid-fluid interface and includes equations to track the evolution of the interface. The Contact Angle subnode is added by default, and is also available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

MODEL INPUT

Enter a value for the **Temperature** T (SI unit: K). This option is only necessary when the surface tension coefficient comes from a library of coefficients, as explained below.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation.

The **Surface tension coefficient** σ (SI unit: N/m) can be **User defined**, or select **Library coefficient, liquid/gas interface** (default) or **Library coefficient, liquid/liquid interface**.

- For **Library coefficient, liquid/gas interface** select an option from the list — **Water/Air** (default), **Acetone/Air**, **Acetic acid/Air**, **Ethanol/Air**, **Ethylene glycol/Ethylene glycol vapor**, **Diethyl ether/Air**, **Glycerol/Air**, **Heptane/Nitrogen**, **Mercury/Mercury vapor**, or **Toluene/Air**.
- For **Library coefficient, liquid/liquid interface** select an option from the list — **Benzene/Water, 20°C**, **Corn oil/Water, 20°C**, **Ether/Water, 20°C**, **Hexane/Water, 20°C**, **Mercury/Water, 20°C**, or **Olive oil/Water, 20°C**.

The predefined correlations are based on the data in Ref. 5, Ref. 6, and Ref. 7.

MASS FLUX

The mass flux setting specifies the mass transfer across the boundary, due to processes such as boiling. The default **Mass Flux** M_f (SI unit: kg/(m^2·s)) is **User defined**, with a value of 0.

NORMAL DIRECTION

The normal direction on the selected boundaries can be reversed by selecting **Reverse normal direction**. The direction is indicated by a red arrow in the Graphics window.

The **Fluid-Fluid Interface** feature imposes a mesh deformation in the normal direction. On adjacent boundaries, the mesh displacement parallel to those boundaries cannot be fixed if the contact point is moving. In this case a Mesh Slip, Symmetry/Roller, Prescribed Normal Mesh Displacement, or Prescribed Normal Mesh Velocity boundary condition under **Definitions>Moving Mesh** should be selected. A Mesh Slip condition is automatically used on boundaries that are adjacent to the Fluid-Fluid Interface and dot not have a prescribed Moving Mesh boundary condition.

If a **Fluid-Fluid Interface** feature is in contact with a solid boundary, the movement of the contact point is not compatible with the no slip condition. For laminar flow the Wall boundary condition with the Navier Slip option should be selected. For turbulence models with wall functions or automatic wall treatment the **Wall** feature with the **No Slip** option can be selected.

Free Surface

The **Free Surface** node defines the initial position of an external fluid interface - that is, an interface in which the viscosity in the fluid outside the domain can be neglected. By applying this feature the motion of the two-phase interface can be tracked. In the tangential direction the free surface motion is governed by the fluid motion in combination with the surface tension of the fluid-fluid interface.

The Free Surface node can only be applied to outer boundaries of a **Deforming Domain** that do not have any boundary condition assigned under **Moving Mesh**.

To control the attachment angle between the free surface and adjacent walls, a Contact Angle subnode is by default added under the **Free Surface** node. A different contact angle subnode can be added from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

The Free Surface feature is supported by laminar flow and by turbulence models using wall functions or automatic wall treatment but not low-Reynolds number wall treatment. It also requires the study to be time dependent. The node is inactive for Frozen Rotor studies.

MODEL INPUT

Enter a value for the **Temperature** T (SI unit: K). This option is only necessary when the surface tension coefficient comes from a library of coefficients, as explained below.

FREE SURFACE

Enter an **External pressure** p_{ext} (SI unit: Pa).

SURFACE TENSION

Select the **Include surface tension force in momentum equation** checkbox to include the surface tension force in the momentum equation.

The default **Surface tension coefficient** σ (SI unit: N/m) can be **User defined**, or select **Library coefficient, liquid/gas interface** (default) or **Library coefficient, liquid/liquid interface**.

- For **Library coefficient, liquid/gas interface** select an option from the list — **Water/Air** (default), **Acetone/Air**, **Acetic acid/Air**, **Ethanol/Air**, **Ethylene glycol/Ethylene glycol vapor**, **Diethyl ether/Air**, **Glycerol/Air**, **Heptane/Nitrogen**, **Mercury/Mercury vapor**, or **Toluene/Air**.
- For **Library coefficient, liquid/liquid interface** select an option from the list — **Benzene/Water, 20°C**, **Corn oil/Water, 20°C**, **Ether/Water, 20°C**, **Hexane/Water, 20°C**, **Mercury/Water, 20°C**, or **Olive oil/Water, 20°C**.

The predefined correlations are based on the data in Ref. 5, Ref. 6, and Ref. 7.

MASS FLUX

The mass flux setting specifies the mass transfer across the boundary, due to processes such as boiling. The default **Mass Flux** M_f (SI unit: kg/(m^2·s)) is **User defined**, with a value of 0.

	The **Free Surface** feature imposes a mesh deformation in the normal direction. On adjacent boundaries, the mesh displacement parallel to those boundaries cannot be fixed if the contact point is moving. In this case a Mesh Slip, Symmetry/Roller, Prescribed Normal Mesh Displacement, or Prescribed Normal Mesh Velocity boundary condition under **Definitions>Moving Mesh** should be selected. A Mesh Slip condition is automatically used on boundaries that are adjacent to the Free Surface and dot not have a prescribed Moving Mesh boundary condition.

	If a **Free Surface** feature is in contact with a solid boundary, the movement of the contact point is not compatible with the no slip condition. For laminar flow the **Wall** boundary condition with the **Navier Slip**option should be selected. For turbulence models with wall functions or automatic wall treatment the **Wall** feature with the **No Slip** option can be selected.

Contact Angle

The **Contact Angle** subnode is available from the context menu (right-click the Fluid-Fluid Interface, Free Surface, or Stationary Free Surface parent node) or from the **Physics** toolbar, **Attributes** menu. The condition applies forces on the wall that balance the surface tension for the prescribed contact angle. Note that the contact angle can only be enforced when the surface tension force is included in the momentum equation in the parent feature.

For laminar flow with moving mesh, the **Contact Angle** node should be used on edges or points where a Wall feature with the **Navier Slip** option is prescribed adjacent to the free surface. In this case, the **Navier Slip** option is required for the contact line to move along the wall.

The representation of the contact angle is dependent on the mesh resolution in the region where the fluid-fluid interface attaches to the wall. If, during the simulation, the contact angle is found to fluctuate around a given value, this indicates that the resolution needs to be improved. This can for example be achieved by adding more mesh boundary layers on the wall.

CONTACT ANGLE

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**.

- For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians.
- For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: $\mathrm{J/m^2}$) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: $\mathrm{J/m^2}$).

NORMAL WALL VELOCITY

Select whether to **Constrain the wall-normal velocity**. This ensures that the fluid velocity normal to the wall on the contact edge or point is exactly the desired value. This can be helpful when the adjacent wall uses a Nitsche Constraints and the no-penetration condition is satisfied in an integral sense rather than pointwise. Moreover, constraining the wall-normal velocity simplifies the equilibrium of forces in the wall-normal direction. This setting should not be selected when the adjacent boundary has an unknown velocity.

The contact angle θ_w is defined between the fluid-fluid interface and the surface of the wall adjacent to phase 1.

The moving mesh boundary condition must be compatible with the motion of the wall for the problem to have a valid solution.

The Bubbly Flow Interfaces

In this section:

- The Laminar Bubbly Flow Interface
- The Bubbly Flow, Algebraic yPlus Interface
- The Bubbly Flow, L-VEL Interface
- The Bubbly Flow, k-ε Interface
- The Bubbly Flow, Realizable k-ε Interface
- The Bubbly Flow, k-ω Interface
- The Bubbly Flow, SST Interface
- The Bubbly Flow, Low Re k-ε Interface
- The Bubbly Flow, Spalart–Allmaras Interface
- The Bubbly Flow, v2-f Interface
- Domain and Boundary Nodes for Bubbly Flow

The Laminar Bubbly Flow Interface

The **Laminar Bubbly Flow (bf)** interface (), found under the **Multiphase Flow** > **Bubbly Flow** branch () when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at low and moderate Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is computed from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density.

The physics interface can also model the distribution of the number density, that is, the number of bubbles per unit volume which in turn can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for laminar bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Laminar Bubbly Flow**, **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Laminar Bubbly Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `bf`.

PHYSICAL MODEL

Specify if the gas concentration is low and whether or not to solve for the interfacial area.

Low Gas Concentration

The **Low gas concentration** checkbox is selected by default. This approximation is valid if the gas volume fraction is low (ϕ_g less than a few percent) and its density does not have any significant effects on the continuity equation. It is then generally valid to replace the continuity equation in The Bubbly Flow Equations; see Equation 6-31 with Equation 6-34).

Solve for Interfacial Area

To add a transport equation for the bubble density in order to determine the interfacial area, select the **Solve for interfacial area** checkbox.

Reference Values

Reference values are global quantities used to evaluate the density of the liquid and the absolute pressure p_A.

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{\text{ref}}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference

pressure level is also used to define the density of the liquid. The default **Reference pressure level** p_{ref} (SI unit: Pa) is 1 atm.

Reference temperature The reference temperature is used to define the density of the liquid. The default **Reference temperature** T_{ref} (SI unit: K) is 293.15 K.

Swirl Flow

For 2D axisymmetric models, select the **Swirl flow** checkbox to include the swirl velocity component — that is, the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction. Also see General Single-Phase Flow Theory in the CFD Module User's Guide.

TURBULENCE

Turbulence Model Type

By default no turbulence model is used.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** u (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: kg/m^3), and the **Number density, gas phase** nd (SI unit: 1/m^3). The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog. Consistent streamline and crosswind diffusion is applied by default to both gas and momentum transport.

Select the **Use dynamic subgrid time scale** checkbox to estimate the influence of temporal variations in the velocity field, instead of using the inverse time step, in the consistent stabilization terms. This checkbox is selected by default

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps.

Additional inconsistent stabilization terms may be added when required as isotropic diffusion. The **Inconsistent Stabilization** section contains the settings for stabilization of the momentum transport (the fluid flow) in the **Momentum transport** area and stabilization of the equation for the dispersed phase in the **Gas phase transport** area.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** checkbox to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable `CFLCMP` which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** $\mathrm{CFL}_{\mathrm{loc}}$ (dimensionless).

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Domain and Boundary Nodes for Bubbly Flow
- Theory for the Bubbly Flow Interfaces

The Bubbly Flow, Algebraic yPlus Interface

The **Bubbly Flow, Algebraic yPlus (bf)** interface ( ), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Algebraic yPlus**.

Wall Treatment

Algebraic yPlus employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

The turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: $\mathrm{kg/m^3}$), the **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$), and the **Wall distance in viscous units** yPlus (dimensionless), and the **Number density, gas phase** nd (SI unit: $1/\mathrm{m^3}$).

The Bubbly Flow, Algebraic yPlus interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Bubbly Flow, L-VEL Interface

The **Bubbly Flow, L-VEL (bf)** interface ( ), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are included using an enhanced viscosity model based on the local wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **L-VEL**.

Wall Treatment

L-VEL employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

The turbulence model parameters are optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** u (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: kg/m^3), the **Reciprocal wall distance** G (SI unit: 1/m), and the **Tangential velocity in viscous units** uPlus (dimensionless), and the **Number density, gas phase** nd (SI unit: $1/m^3$).

The Bubbly Flow, L-VEL interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Bubbly Flow, k-ε Interface

The **Bubbly Flow, k-ε(bf)** interface ( ), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints and bubble-induced turbulence production. The flow near walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **k-ε**.

Wall Treatment

Wall treatment for the k-ε model can only be set to **Wall functions**. More options become available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: $\mathrm{kg/m^3}$), the **Turbulent dissipation rate** ep (SI unit: $\mathrm{m^2/s^3}$), the **Turbulent kinetic energy** k (SI unit: $\mathrm{m^2/s^2}$), and the **Number density, gas phase** nd (SI unit: $\mathrm{1/m^3}$).

The names of variables can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog. The settings for this section are the same as for The Laminar Bubbly Flow Interface with the addition of this section: stabilization for the turbulence variables in the **Turbulence equations** area.

When using a turbulence model, streamline and crosswind diffusion are by default applied to the turbulence equations.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. The **Turbulence variables scale parameters** subsection is available when the **Turbulence model type** is set to **RANS-EVM**.

In addition to the settings described for The Laminar Bubbly Flow Interface, enter a value for U_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The U_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units, or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver.

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Domain and Boundary Nodes for Bubbly Flow
- Theory for the Bubbly Flow Interfaces

Flow in an Airlift Loop Reactor: Application Library path **CFD_Module/Verification_Examples/airlift_loop_reactor**

The Bubbly Flow, Realizable k-ε Interface

The **Bubbly Flow, Realizable k-ε(bf)** interface ( ), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the

realizable two-equation k-ε model and bubble-induced turbulence production. The flow near walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-$\mathcal{E}$ Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Realizable k-ε**.

Wall Treatment

Wall treatment for the Realizable k-ε model can only be set to **Wall functions**. More options becomes available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: $\mathrm{kg/m^3}$), the **Turbulent dissipation rate** ep (SI unit: $\mathrm{m^2/s^3}$), the **Turbulent kinetic energy** k (SI unit: $\mathrm{m^2/s^2}$), and the **Number density, gas phase** nd (SI unit: $\mathrm{1/m^3}$).

The Bubbly Flow, k-ω Interface

The **Bubbly Flow, k-ω (bf)** interface ( ), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the Wilcox revised two-equation k-ω model with realizability constraints and bubble-induced turbulence production. The k-ω model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **k-ω**.

Wall Treatment

The k-ω model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. The most robust, but least accurate option is select the **Wall functions** option.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough. Observe that the **Low Re** formulation requires the wall distance to be solved for prior to the flow.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: $\mathrm{kg/m^3}$), the **Specific dissipation rate** om (SI unit: 1/s), the **Turbulent kinetic energy** k (SI unit: $\mathrm{m^2/s^2}$), and the **Number density, gas phase** nd (SI unit: $\mathrm{1/m^3}$).

The Bubbly Flow, SST Interface

The **Bubbly Flow, SST (bf)** interface (), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch () when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability constraints and bubble-induced turbulence production. The SST model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **SST**.

Wall Treatment

The SST model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: $\mathrm{kg/m^3}$), the **Specific dissipation rate** om (SI unit: 1/s), the **Turbulent kinetic energy** k (SI unit: $\mathrm{m^2/s^2}$), the **Reciprocal wall distance** G (SI unit: 1/m), and the **Number density, gas phase** nd (SI unit: $\mathrm{1/m^3}$).

The Bubbly Flow, SST interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Bubbly Flow, Low Re k-ε Interface

The **Bubbly Flow, Low Re k-ε (bf)** interface (), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch () when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the AKN two-equation k-ε with realizability constraints and bubble-induced turbulence production. The AKN model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Low Reynolds number k-ε**.

Wall Treatment

The AKN model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** `rhogeff` (SI unit: kg/m^3), the **Turbulent dissipation rate** `ep` (SI unit: m^2/s^3), the **Turbulent kinetic energy** k (SI unit: m^2/s^2), the **Reciprocal wall distance** G (SI unit: $1/m$), and the **Number density, gas phase** `nd` (SI unit: $1/m^3$).

The Bubbly Flow, Low Re k-ε interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

The Bubbly Flow, Spalart–Allmaras Interface

The **Bubbly Flow, Spalart–Allmaras (bf)** interface ( ), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch ( ) when adding a physics

interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the Spalart–Allmaras one-equation model. The Spalart–Allmaras model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The Spalart–Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Spalart–Allmaras**.

Wall Treatment

The Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: $\mathrm{kg/m^3}$), the **Undamped turbulent kinematic viscosity** nutilde (SI unit: $\mathrm{m^2/s}$), the **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$), and the **Number density, gas phase** nd (SI unit: $1/\mathrm{m^3}$).

The Bubbly Flow, Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual.*

The Bubbly Flow, v2-f Interface

The **Bubbly Flow, v2-f (bf)** interface ( ), found under the **Multiphase Flow** > **Bubbly Flow** > **Bubbly Flow, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier–Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the v2-f transport-equation model with realizability constraints and bubble-induced turbulence production. The v2-f model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The v2-f model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **v2-f**.

Wall Treatment

The v2-f model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field, liquid phase u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: kg/m^3), the **Turbulent dissipation rate** ep (SI unit: m^2/s^3), the **Turbulent kinetic energy** k (SI unit: m^2/s^2), the **Turbulent relative fluctuations** zeta (dimensionless), the **Elliptic**

blending function alpha (dimensionless), the **Reciprocal wall distance** G (SI unit: 1/m), and the **Number density, gas phase** nd (SI unit: $1/m^3$).

The Bubbly Flow, v2-f interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

Domain and Boundary Nodes for Bubbly Flow

The following domain and boundary nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

DOMAIN

- Fluid Properties
- Volume Force (described for The Laminar Flow Interface)
- Mass Transfer
- Gravity
- Initial Values

BOUNDARY

The sections describe the available boundary conditions for the liquid and the gas. In all equations, **n** denotes the outward pointing unit vector normal to the boundary.

The boundary types for the liquid flow variables, described in this section, are:

- Wall (the default boundary condition)
- Inlet
- Outlet

- Symmetry
- Periodic Flow Condition
- Interior Wall

PAIR

- Flow Continuity

In addition to the boundary conditions for the liquid, the following boundary conditions for the gas are available for all boundary condition types except symmetry and interior wall:

- Gas Concentration (the default condition for inlets)
- Gas Flux
- Gas Outlet (the default condition for outlets)
- No Gas Flux (the default condition for walls)
- Symmetry

Gas Boundary Condition Equations

For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Fluid Properties

The **Fluid Properties** node contains the material properties for the liquid and the gas. It also contains settings for the slip model.

MODEL INPUTS

Fluid properties, such as the gas density and liquid viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The default **Absolute pressure** p_A is $p+p_{\mathrm{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIALS

Select the materials to use for the material properties of the liquid and the gas (when they are set to take their value from the material). The default is to use the **Domain material** for the **Liquid** and **None** for the **Gas**. Select another material to use that material's properties for the liquid or gas as needed.

LIQUID PROPERTIES

The default **Density, liquid phase** ρ_l (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref}, which are specified at the physics interface level.

The default **Dynamic viscosity, liquid phase** μ_l (SI unit: Pa·s) uses values **From material**; the value is then defined for the material selected in the **Materials** section for the continuous phase. For **User defined** enter another value or expression.

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity.

GAS PROPERTIES

The default **Density, gas phase** ρ_g (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression. Alternatively, select **Calculate from ideal gas law** and enter the **Molecular weight** M (SI unit: kg/mol) of the gas.

Enter the **Bubble diameter** d_b (SI unit: m). The default value is 10^{-3} m (1 mm).

SLIP MODEL

Select a **Slip model** — **Homogeneous flow** (the default), **Pressure-drag balance**, or **User defined**.

Homogeneous flow assumes that the velocity of the two phases are equal; that is, $\mathbf{u}_{slip} = 0$. For **User defined** enter different values or expressions for the components of the **Slip velocity** $\mathbf{u}_{slip}$ (SI unit: m/s).

For **Pressure-drag balance** it uses a model based on the assumption that the pressure forces on a bubble are balanced by the drag force:

$$\frac{3}{4}\frac{C_d}{d_b}\rho_l|\mathbf{u}_{slip}|\mathbf{u}_{slip} = -\nabla p$$

Here d_b (SI unit: m) is the bubble diameter, and C_d (dimensionless) is the drag coefficient.

Select a **Drag coefficient model**:

- **Small spherical bubbles (Hadamard-Rybczynski)** for bubbles with a diameter smaller than 2 mm.
- **Large bubbles** for gas bubbles with a diameter larger than 2 mm. Then enter the **Surface tension coefficient** σ (SI unit N/m). The default is 0.07 N/m.
- **Air bubbles in tap water (Schwarz-Turner)** for air bubbles of 1–10 mm mean diameter in water.
- **User defined** to enter a different value or expression for the **Drag coefficient** C_d (dimensionless). The default value is 1.

See the Slip Model theory section.

MIXING LENGTH LIMIT

This section is available for the Bubbly Flow, k-ε, Bubbly Flow, Realizable k-ε, and Bubbly Flow, k-ω interfaces, where an upper limit on the mixing length is required.

When the **Mixing length limit** $l_{\mathrm{mix,lim}}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression.

DISTANCE EQUATION

This section is available for the Bubbly Flow, Low Re k-ε, Bubbly Flow, Algebraic yPlus, Bubbly Flow, L-VEL, Bubbly Flow, SST, Bubbly Flow, Spalart–Allmaras, and Bubbly Flow, v2-f interfaces.

When the **Reference length scale** l_{ref} is set to **Automatic**, it is evaluated one tenth of the shortest side of the geometry bounding box. The solution to the wall distance equation is controlled by the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling because small objects would have too large an impact on the solution if the wall distance were measured exactly. The automatic value is usually a good choice but the value can become too high if the geometry consists of several slim

entities. In such cases, it is recommended that the reference length scale is defined manually. Select **Manual** to enter a different value or expression.

Mass Transfer

Add a **Mass Transfer** node to include mass transfer from the gas to the liquid.

MASS TRANSFER

Select a **Mass transfer model** — **Two-film theory**, **Nonequilibrium model**, or **User defined**. For **User defined** enter a value or expression for the **Mass transfer from gas to liquid** m_{gl} (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

Nonequilibrium Model

For **Nonequilibrium model** enter values or expressions for each of the following:

- **Equilibrium volume fraction in dispersed phase** ϕ_{eq}. The default is 0.
- **Inverse time scales** f_l and f_g (SI unit: 1/s). The default is 0 s^{-1}.

The mass transfer is modeled as

$$m_{gl} = \rho_g[f_l \max(\phi_g - \phi_{eq}) - f_g \max(\phi_{eq} - \phi_g)]$$

Two-Film Theory

For **Two-film theory** enter values for the **Mass transfer coefficient** k (SI unit: m/s), **Henry's constant** H (SI unit: Pa·m^3/mol), the **Dissolved gas concentration** c (SI unit: mol/m^3), and the **Molecular weight of species** M (SI unit: kg/mol). Refer to the theory below for more information.

Henry's law gives the equilibrium concentration c^* of gas dissolved in liquid:

$$c^* = \frac{p + p_{ref}}{H}$$

where H is Henry's constant. The molar flux per interfacial area, N (SI unit: mol/(s·m^2)), is determined by

$$N = k(c^* - c)$$

where k is the Mass transfer coefficient and c is the Dissolved gas concentration in liquid.

The mass transfer from gas to liquid, m_{gl}, is given by

$$m_{\mathrm{gl}} = NMa$$

where M is the Molecular weight of species and a is the interfacial area per volume (SI unit: $\mathrm{m}^2/\mathrm{m}^3$).

Also see Theory for the Bubbly Flow Interfaces for details about how a is computed.

For two-film theory, you also need to solve for the concentration of the dissolved gas;

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}_{\mathrm{l}}) = \nabla \cdot (D\nabla c) + \frac{m_{\mathrm{gl}}}{M}$$

which can be done by adding a Transport of Diluted Species interface.

Gravity

The **Gravity** node adds the force $\rho\mathbf{g}$ to the right-hand side of the momentum transport equation. Gravity nodes are mutually exclusive, that is, there can only be one active Gravity node per domain.

GRAVITY

Enter the components of the **Gravity vector**, $\mathbf{g}$ (SI unit: $\mathrm{m/s}^2$). For 2D components the default Gravity vector is defined as (0, –g_const). Here g_const is a physical constant equal to 9.8066 $\mathrm{m/s}^2$. For 3D and 2D axisymmetric components, the gravity acts in the negative z direction by default.

Initial Values

The **Initial Values** node adds initial values for the flow variables and the effective gas density that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field, liquid phase** $\mathbf{u}$ (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0. Also enter a value or expression for the **Effective gas density** rhogeff (SI unit: $\mathrm{kg/m}^3$). The default is 0 $\mathrm{kg/m}^3$.

If the **Solve for interfacial area** checkbox is selected, enter an initial value for the **Number density, gas phase** nd (SI unit: $1/m^3$). The default is 0 $1/m^3$.

For the Bubbly Flow, Turbulent Flow interfaces, initial values for the turbulence variables should be also specified. Additional initial values may be required for:

- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep
- **Reciprocal wall distance** G
- **Specific dissipation rate** om
- **Undamped turbulent kinematic viscosity** υ_0
- **Wall distance in viscous units** yPlus
- **Tangential velocity in viscous units** uPlus
- **Turbulent relative fluctuations** zeta
- **Elliptic blending function** alpha

Wall

The **Wall** node adds a selection of boundary conditions that describe the existence of a solid wall. The Wall node by default specifies no gas flux for the gas phase.

Gas Boundary Condition Equations

LIQUID BOUNDARY CONDITION

Select a **Liquid boundary condition** — **No slip** (the default) or **Slip**.

No Slip

No slip is the default boundary condition for the liquid. A no slip wall is a wall where the liquid velocity relative to the wall velocity is zero. For stationary walls, it sets the liquid velocity to zero at the wall:

$$\mathbf{u}_l = 0$$

For turbulent bubbly flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall functions** are selected, the **Apply wall roughness** option becomes available. Click to select the **Apply wall roughness** checkbox to apply the roughness correction. When the checkbox is selected, the default **Roughness model** is **Sand roughness**, which is derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

- For **Sand roughness** enter an **Equivalent sand roughness height** k_{seq} (SI unit: m). The default is 3.2 micrometers.
- For **Generic roughness** enter a **Roughness height** k_{s} (SI unit: m). The default is 3.2 micrometers. Then enter a **Roughness parameters** C_{s} (dimensionless). The default is 0.26.

References for the Single-Phase Flow, Turbulent Flow Interfaces

Slip

Sets the velocity component normal to the wall to zero:

$$\mathbf{u}_{\mathrm{l}} \cdot \mathbf{n} = 0$$

GAS BOUNDARY CONDITION

From the list, select a **Gas boundary condition** for the gas phase on the wall — **No gas flux** (the default), **Gas concentration**, **Gas outlet**, **Gas flux**, or **Symmetry**.

Gas Concentration

For **Gas concentration** enter the **Effective gas density** $\rho_{\mathrm{g}}\phi_{\mathrm{g0}}$ (SI unit: kg/m^3). The default is 0 kg/m^3.If **Solve for interfacial area** is selected, also select either the **Bubble number density** (the default) or the **Bubble diameter and gas density** button.

- For **Bubble number density** enter the **Bubble number density** n_0 (SI unit: 1/m^3). The default is 1000 1/m^3.
- For **Bubble diameter and gas density** enter the **Bubble diameter** d_{b} (SI unit: m) (the default is 1 mm) and **Density, gas phase** ρ_{g} (SI unit: kg/m^3) (the default is 1 kg/m^3).

Gas Flux

For **Gas flux** enter the **Gas mass flux** $N_{\rho_g\phi_g}$ (SI unit: kg/(m^2·s)) (the default is 0 kg/(m^2·s)) and if the **Solve for interfacial area** checkbox is selected on the physics interface, the **Number density flux** N_{n} (SI unit: 1/(m^2·s)). The default is 0 (1/(m^2·s)).

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the spatial frame.

The **Translational velocity** setting controls the translational velocity, $\mathbf{u}_{tr}$. The list is per default set to **Automatic from frame**. When **Automatic from frame** is selected, the physics automatically detects if the spatial frame moves. If there is no movement, $\mathbf{u}_{tr}$ is set to $\mathbf{0}$. If the frame moves, $\mathbf{u}_{tr}$ becomes equal to the frame movement. $\mathbf{u}_{tr}$ is accounted for in the actual boundary condition prescribed in the **Liquid boundary condition** section.

When **Manual** is selected from **Translational velocity** selection list, the **Velocity of moving wall**, $\mathbf{u}_{tr}$ can be prescribed manually. Specifying the translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options.**

	Wall in the Single-Phase Flow interfaces

Inlet

The **Inlet** node adds a selection of boundary conditions that describe inlets in fluid-flow simulations.

	Gas Boundary Condition Equations

LIQUID BOUNDARY CONDITION

Select a **Liquid boundary condition** — **Velocity** (the default), **Pressure**, or **Fully developed flow**.

VELOCITY

For **Velocity** click the **Normal inflow velocity** (the default) or **Velocity field** buttons.

- For **Normal inflow velocity** enter a value or expression for U_0 (SI unit: m/s).
- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{u}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{u}_1 = \mathbf{u}_0$$

PRESSURE

This condition specifies the normal stress which in most cases is approximately equal to the pressure. Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.

- The **Suppress backflow** checkbox is selected by default. This option adjusts the inlet pressure, $\hat{p}_0 \geq p_0$, locally in order to reduce the amount of fluid exiting the domain through the boundary. If suppress backflow is deselected, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.
- **Flow direction** controls in which direction the fluid enters the domain.
  - For **Normal flow** (the default) it prescribes zero tangential velocity component.
  - For **User defined** define an **Inflow velocity direction**, $\mathbf{d}_\mathbf{u}$ (dimensionless). The magnitude of $\mathbf{d}_\mathbf{u}$ does not matter, only the direction. $\mathbf{d}_\mathbf{u}$ must point into the domain.

FULLY DEVELOPED FLOW

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow toward the solution for a fully developed channel flow. The channel can be thought of as a virtual extrusion of the inlet cross section. The velocity is defined by the boundary condition of the adjacent boundary in the model.

The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the inlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

Select a **Fully developed flow** option — **Average velocity** (the default), **Flow rate**, or **Average pressure**.

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow toward the solution for a fully developed channel flow.

Select an option to control the flow rate at the inlet:

- For **Average velocity** enter U_{av}.
- **Flow rate**, V_0. Two-dimensional models also require an **Entrance thickness**, D_z, which is the out-of-plane thickness of the extruded entrance channel.
- **Average pressure**, P_{av}. Observe that P_{av} is the average pressure on the inflow boundary.

Fully developed inflow can be used in conjunction with the turbulence models. No additional inputs are required for the turbulence variables. They are instead solved for on the inlet boundary to be consistent with the fully developed flow profile.

A fully developed flow boundary cannot be adjacent to any Interior Wall feature

GAS BOUNDARY CONDITION

These settings are the same as for Wall. See Gas Boundary Condition. The only difference is that **Gas concentration** is the default.

TURBULENCE CONDITIONS

This section is available for Bubbly Flow, Turbulent Flow interfaces. No additional inputs are required for **Fully developed flow**.

No additional inlet conditions are required for the algebraic turbulence models: Algebraic yPlus and L-VEL.

For the **Bubbly Flow, Spalart–Allmaras** interface, a value or expression for the **Undamped turbulent kinematic viscosity** ν_0 should be specified. The default value is `3*bf.nul`.

For transport-equation turbulence models, apart from Spalart–Allmaras, the following settings are available under the **Specify turbulence length scale and intensity** option (see Table 3-3 for the default values):

- **Turbulent intensity** I_{T}
- **Turbulent length scale** L_{T}
- **Reference velocity scale** U_{ref}

For the v2-f turbulence model, the additional choice between **Isotropic turbulence** and **Specify turbulence anisotropy** appears. For **Specify turbulence anisotropy**, a value for the turbulent relative fluctuations at the inlet, ζ_0, may be specified. When **Specify turbulence variables** is selected, values or expressions for the dependent turbulence

variables should be defined. Availability is based on the physics interface and the boundary condition chosen.

- **Turbulent kinetic energy** k_0
- **Turbulent dissipation rate**, ε_0
- **Specific dissipation rate** ω_0
- **Turbulent relative fluctuations** ζ_0
- **Elliptic blending function** α_0

The turbulent length scale L_T and turbulence intensity I_T are related to the turbulence variables, see Theory for the Turbulent Flow Interfaces.

See Inlet in the Single-Phase Flow interfaces

Outlet

The **Outlet** node adds a set of boundary conditions that describe outlets in fluid-flow simulations; that is, the conditions at boundaries where the fluid exits the domain.

LIQUID BOUNDARY CONDITION

Select a **Liquid boundary condition** — **Pressure** (the default), **Velocity**, or **Fully developed flow**.

PRESSURE CONDITIONS

The **Pressure** condition specifies the normal stress which in most cases is approximately equal to the pressure. The tangential stress component is set to 0 $\mathrm{N/m^2}$.

- Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.
- Select the **Normal flow** checkbox to change the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The **Suppress backflow** checkbox is selected by default. This option adjusts the outlet pressure in order to reduce the amount of fluid entering the domain through the boundary.

VELOCITY

For **Velocity** click the **Velocity field** (the default) or **Normal outflow velocity** buttons.

- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{u}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{u}_1 = \mathbf{u}_0$$

- For **Normal outflow velocity** enter a value or expression for U_0 (SI unit: m/s).

FULLY DEVELOPED FLOW

This boundary condition is applicable when the flow exits the domain into a long pipe or channel, at the end of which a flow profile is fully developed.

The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the outlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

Select a **Fully developed flow option** — **Average velocity** (the default), **Flow rate**, or **Average pressure**.

GAS BOUNDARY CONDITION

The settings for the **Gas boundary condition** are the same as for Wall. See Gas Boundary Condition.

When the **Gas boundary condition** is set to **Gas outlet**, the **Exterior gas condition(s)** section contains an input field for the **Effective gas density** on the downstream side of the outlet. If **Solve for interfacial area** is selected at the physics interface level, additional input fields appear for the **Bubble number density** or the **Bubble diameter and gas density** on the downstream side of the outlet.

See Outlet in the Single-Phase Flow interfaces

Symmetry

The **Symmetry** node adds boundary conditions that describe symmetry boundaries in fluid-flow simulations. The boundary condition for symmetry boundaries prescribes no penetration and vanishing shear stresses:

$$\mathbf{u}_1 \cdot \mathbf{n} = 0, \qquad \mathbf{t}^T\left(\phi_1(\mu_1 + \mu_T)\left(\nabla \mathbf{u}_1 + \nabla \mathbf{u}_1{}^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_1)\mathbf{I}\right)\right)\mathbf{n} = 0$$

BOUNDARY SELECTION

A boundary condition for 2D axial symmetry is not required.

For the symmetry axis at $r = 0$, the software automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the z direction and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group. Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

PRESSURE DIFFERENCE

A value or expression should be specified for the **Pressure difference**, $p_{\text{src}} - p_{\text{dst}}$. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** section is available when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Flow Condition** node.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options** in the **Show More Options** dialog.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation**

of Source section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Interior Wall

The **Interior Wall** node adds a wall boundary condition on interior boundaries. It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall node specifies no gas flux for the gas phase.

Gas Boundary Condition Equations

LIQUID BOUNDARY CONDITION

Select a **Liquid boundary condition** — **No slip** (the default) or **Slip**.

No Slip

No slip is the default boundary condition for the liquid. A no slip wall is a wall where the liquid velocity relative to the wall velocity is zero. For interior stationary walls, it sets the liquid velocity to zero on both sides of the wall:

$$\mathbf{u}_l = 0$$

For turbulent bubbly flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

Slip

The **Slip** condition prescribes a no-penetration condition. For an interior stationary wall it sets the velocity component normal to the interior wall to zero on both sides of the wall:

$$\mathbf{u}_l \cdot \mathbf{n} = 0$$

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the spatial frame.

The **Translational velocity** setting controls the translational velocity, $\mathbf{u}_{tr}$. The list is per default set to **Automatic from frame**. When **Automatic from frame** is selected, the physics automatically detects if the spatial frame moves. If there is no movement, $\mathbf{u}_{tr}$ is set to $\mathbf{0}$. If the frame moves, $\mathbf{u}_{tr}$ becomes equal to the frame movement. $\mathbf{u}_{tr}$ is accounted for in the actual boundary condition prescribed in the **Liquid boundary condition** section.

When **Manual** is selected from **Translational velocity** selection list, the **Velocity of moving wall**, $\mathbf{u}_{tr}$ can be prescribed manually. Specifying the translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options.**

	Wall

Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the Wall node is used as fallback unless another feature has been selected for the boundary.

	About Pairs

Gas Boundary Condition Equations

In addition to the boundary conditions for the liquid, specify boundary conditions for the gas on Wall, Inlet, Outlet, and Interior Wall nodes. Select a **Gas Boundary Condition**:

Gas Concentration

Using this boundary condition, specify the effective gas density.

$$\tilde{\rho}_g = \tilde{\rho}_g^0$$

Gas Outlet

This boundary condition is appropriate for boundaries where the gas phase flows outward with the gas velocity, $\mathbf{u}_g$, at the boundary.

Gas Flux

Using this boundary condition, specify the gas mass flux through the boundary:

$$-\mathbf{n} \cdot (\tilde{\rho}_g \mathbf{u}_g) = N_{\rho_g \phi_g}$$

Symmetry

This boundary condition, which is useful on boundaries that represent a symmetry line for the gas flow, sets the gas flux through the boundary to zero:

$$\mathbf{n} \cdot (\tilde{\rho}_g \mathbf{u}_g) = 0$$

No Gas Flux

This boundary condition represents boundaries where the gas flux through the boundary is zero:

$$\mathbf{n} \cdot (\phi_g \mathbf{u}_g) = 0$$

In walls moving with a boundary velocity $\mathbf{u}_{\text{bnd}}$, the gas flux through the boundary is:

$$\mathbf{n} \cdot (\phi_g \mathbf{u}_g) = \mathbf{n} \cdot (\phi_g \mathbf{u}_{\text{bnd}})$$

The Mixture Model Interfaces

In this section:

- The Mixture Model, Laminar Flow Interface
- The Mixture Model, Algebraic yPlus Interface
- The Mixture Model, L-VEL Interface
- The Mixture Model, k-ε Interface
- The Mixture Model, Realizable k-ε Interface
- The Mixture Model, k-ω Interface
- The Mixture Model, SST Interface
- The Mixture Model, Low Re k-ε Interface
- The Mixture Model, Spalart–Allmaras Interface
- The Mixture Model, v2-f Interface
- Domain and Boundary Nodes for the Mixture Model Interfaces

The Mixture Model, Laminar Flow Interface

The **Mixture Model, Laminar Flow (mm)** interface (), found under the **Multiphase Flow** > **Mixture Model** branch () when adding a physics interface, is used to model the flow at low and moderate Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Laminar Flow interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

The main physics node is the Mixture Properties feature. It adds the equations for the mixture and provides an interface for defining the fluid materials for the continuous and dispersed phases as well as which slip model and mixture viscosity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Mixture Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Mixture Model, Laminar Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `mm`.

PHYSICAL MODEL

Specify the characteristics of the dispersed phase, the model for the slip velocity, and whether or not to solve for the interfacial area.

Dispersed Phase

To characterize the **Dispersed phase**, select **Solid particles** (the default) or **Liquid droplets/bubbles**.

The selection from this list is further defined for the Mixture Properties node under the Mixture Model section.

Slip Model

To compute the slip velocity $\mathbf{j}_{\text{slip}}$ (SI unit: m/s), select a **Slip model** — **Homogeneous flow** (the default), **Hadamard-Rybczynski**, **Schiller-Naumann**, **Haider-Levenspiel**, or **User defined**.

- The **Homogeneous flow** model assumes that the velocities of the two phases are equal, that is, $\mathbf{u}_{\text{slip}} = 0$.
- In most cases there is a significant difference in the velocity fields due to the buoyancy of the dispersed phase. Use one of the predefined slip models for such cases.
- For **User defined** specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data. Enter the **Slip velocity field** $\mathbf{u}_{\text{slip}}$

(SI unit: m/s) or **Slip flux** $\mathbf{j}_{\text{slip}}$ (SI unit: m/s) in the Mixture Properties node under the Mixture Model section.

Solve For Interfacial Area

To add a transport equation for the number density of the dispersed particles, in order to determine the interfacial area, select the **Solve for interfacial area** checkbox (by default not selected).

For the Mass Transfer rate, use a two-film theory model, which includes the interfacial area per unit volume between the two phases. It is possible to compute the interfacial area per unit volume if the number density n (that is, the number of dispersed particles per volume) is known. Select the **Solve for interfacial area** checkbox to add the following equation for the number density n:

$$\frac{\partial n}{\partial t} + \mathbf{j} \cdot \nabla n + \nabla \cdot (n \mathbf{u}_{slip} \phi_c) = 0$$

This equation states that a dispersed phase particle cannot disappear, appear, or merge with other particles, although it can expand or shrink.

The Mixture Model, Laminar Flow Interface calculates the interfacial area a (SI unit: m^2/m^3) from

$$a = (4n\pi)^{1/3}(3\phi_{\text{d}})^{2/3}$$

Reference values

Reference values are global quantities used to evaluate the density of both phases and the absolute pressure p_A.

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{\text{ref}}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the density of both phases. The default **Reference pressure level** p_{ref} (SI unit: Pa) is `1[atm]`.

Reference temperature The reference temperature is used to define the density of both phases. The default **Reference temperature** T_{ref} (SI unit: K) is `293.15[K]`.

Swirl Flow

For 2D axisymmetric components, select the **Swirl flow** checkbox to include the swirl velocity component — that is, the velocity component j_φ in the azimuthal direction. While j_φ can be nonzero, there can be no gradients in the φ direction.

General Single-Phase Flow Theory

TURBULENCE

Turbulence Model Type

The default selection is **None**.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$).

The names can be changed but the names of fields and dependent variables must be unique within a component.

In previous versions of COMSOL Multiphysics (prior to version 5.4), the Mixture Model interfaces solved for the mass-averaged mixture velocity **u**. Now, the volume-averaged mixture velocity **j** is used. For specific details, see Theory for the Mixture Model Interfaces and Mass-Averaged Mixture Velocity.

CONSISTENT STABILIZATION AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

The consistent stabilizations **Streamline diffusion** and **Crosswind diffusion** are by default applied to the **Navier-Stokes and dispersed phase transport equations**. In addition, when the flow is turbulent, the consistent stabilizations are also applied to the **Turbulence**.

Additional inconsistent stabilization terms may be added when required as isotropic diffusion.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Penalty Diffusion can be used to suppress negative values of the dispersed volume fraction. Including this term has been observed to slow down convergence and it is therefore disabled by default.

Select the **Use pseudo time stepping for stationary equation form** checkbox to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable `CFLCMP` which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** $\mathrm{CFL}_{\mathrm{loc}}$ (dimensionless).

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Domain and Boundary Nodes for the Mixture Model Interfaces
- The Mixture Model, k-ε Interface
- Slip Velocity Models and Theory for the Mixture Model Interfaces

Two-Phase Flow Modeling of a Dense Suspension: Application Library path **CFD_Module/Verification_Examples/dense_suspension**

The Mixture Model, Algebraic yPlus Interface

The **Mixture Model, Algebraic yPlus (mm)** interface ( ), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Algebraic yPlus interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are included using and enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Algebraic yPlus**.

Wall Treatment

Algebraic yPlus employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)

- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$)
- **Wall distance in viscous units** yPlus (dimensionless)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, Algebraic yPlus interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, L-VEL Interface

The **Mixture Model, L-VEL (mm)** interface (), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch () when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, L-VEL interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation, and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are included using and enhanced viscosity model based on the local wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **L-VEL**.

Wall Treatment

L-VEL employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$)
- **Tangential velocity in viscous units** uPlus (dimensionless)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, L-VEL interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, k-ε Interface

The **Mixture Model, k-ε (mm)** interface ( ), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, k-ε interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **k-ε**.

Wall Treatment

Wall treatment for the k-ε model can only be set to **Wall functions**. More options become available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Turbulent kinetic energy** k (SI unit: $\mathrm{m}^2/\mathrm{s}^2$)
- **Turbulent dissipation rate** ε (SI unit: $\mathrm{m}^2/\mathrm{s}^3$)

The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization**. The settings for this section are the same as for The Mixture Model, Laminar Flow Interface with the addition of this section: stabilization for the turbulence variables in the **Turbulence equations** area.

When using a turbulence model, streamline and crosswind diffusion are by default applied to the turbulence equations.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**. The **Turbulence variables scale parameters** subsection is available when the **Turbulence model type** is set to **RANS-EVM** or **RANS-RSM**.

In addition to the settings described for The Mixture Model, Laminar Flow Interface, enter a value for J_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The J_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units,

or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver.

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, Realizable k-ε Interface

The **Mixture Model, Realizable k-ε (mm)** interface (), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch () when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Realizable k-ε interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the realizable two-equation k-ε model. Flow close to walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Realizable k-ε**.

Wall Treatment

Wall treatment for the Realizable k-ε model can only be set to **Wall functions**. More options become available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Turbulent kinetic energy** k (SI unit: $\mathrm{m}^2/\mathrm{s}^2$)
- **Turbulent dissipation rate** ε (SI unit: $\mathrm{m}^2/\mathrm{s}^3$)

The names can be changed but the names of fields and dependent variables must be unique within a component.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, k-ω Interface

The **Mixture Model, Realizable k-ω (mm)** interface ( ), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, k-ω interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture

averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Wilcox revised two-equation k-ω model with realizability constraints. The k-ω model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **k-ω**.

Wall Treatment

The k-ω model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. The most robust, but least accurate option is to select the **Wall functions** option.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough. Observe that the **Low Re** formulation requires the wall distance to be solved for prior to the flow.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)

- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Turbulent kinetic energy** k (SI unit: $\mathrm{m}^2/\mathrm{s}^2$)
- **Specific dissipation rate** ω (SI unit: $1/\mathrm{s}$)

The names can be changed but the names of fields and dependent variables must be unique within a component.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, SST Interface

The **Mixture Model, SST (mm)** interface (), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch () when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, SST interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability constraints. The SST model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **SST**.

Wall Treatment

The SST model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture** **j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$)
- **Turbulent kinetic energy** k (SI unit: $\mathrm{m}^2/\mathrm{s}^2$)
- **Specific dissipation rate** ω (SI unit: $1/\mathrm{s}$)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, SST interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, Low Re k-ε Interface

The **Mixture Model, Low Re k-ε (mm)** interface (), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch () when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Low Re k-ε interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the AKN two-equation k-ε model with realizability constraints. The AKN model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Low Reynolds number k-ε**.

Wall Treatment

The AKN model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture** **j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$)
- **Turbulent kinetic energy** k (SI unit: $\mathrm{m}^2/\mathrm{s}^2$)
- **Turbulent dissipation rate** ε (SI unit: $\mathrm{m}^2/\mathrm{s}^3$)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, Low Re k-ε interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, Spalart–Allmaras Interface

The **Mixture Model, Spalart–Allmaras (mm)** interface ( ), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Spalart–Allmaras interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Spalart–Allmaras one-equation model. The Spalart–Allmaras model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The Spalart–Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Spalart–Allmaras**.

Wall Treatment

The Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$)
- **Undamped turbulent kinematic viscosity** nutilde (SI unit: m^2/s)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

The Mixture Model, v2-f Interface

The **Mixture Model, v2-f (mm)** interface ( ), found under the **Multiphase Flow** > **Mixture Model** > **Mixture Model, Turbulent Flow** branch ( ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, v2-f interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the v2-f transport-equation model with realizability constraints. The v2-f model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The v2-f model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-ε Interface.

TURBULENCE

The default **Turbulence model type** is **RANS-EVM**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **v2-f**.

Wall Treatment

The v2-f model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- **Velocity field, mixture j** (SI unit: m/s)
- **Pressure** p (SI unit: Pa)
- **Volume fraction, dispersed phase** phid (dimensionless)
- **Squared slip velocity** slipvel
- **Number density, dispersed phase** nd (SI unit: $1/\mathrm{m}^3$)
- **Reciprocal wall distance** G (SI unit: $1/\mathrm{m}$)
- **Turbulent kinetic energy** k (SI unit: $\mathrm{m}^2/\mathrm{s}^2$)
- **Turbulent dissipation rate** ε (SI unit: $\mathrm{m}^2/\mathrm{s}^3$)
- **Turbulent relative fluctuations** zeta (dimensionless)
- **Elliptic blending function** alpha (dimensionless)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, v2-f interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the *COMSOL Multiphysics Reference Manual*.

- Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models
- Theory for the Mixture Model Interfaces

Domain and Boundary Nodes for the Mixture Model Interfaces

The following domain and boundary nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

DOMAIN

- Mixture Properties
- Mass Transfer
- Volume Force (described for The Laminar Flow Interface)
- Gravity
- Initial Values

BOUNDARY

The boundary types for the mixture flow variables, described in this section, are:

- Wall (the default boundary condition feature)
- Inlet
- Outlet
- Symmetry
- Periodic Flow Condition
- Interior Wall

PAIR

- Mixture Continuity

For the flow variables, the velocity and the pressure, the boundary conditions correspond to those defined for single phase flow (see Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow). There is also a point constraint for the pressure, which is useful if no other boundary condition in the model includes a pressure level constraint.

The following boundary conditions for the dispersed phase are available for all boundary condition types except symmetry and interior wall. These are described in more detail in the Theory for the Mixture Model Interfaces.

- **Dispersed phase concentration** (the default condition for inlets)
- **Dispersed phase flux**
- **Dispersed phase outlet** (the default condition for outlets)
- **No dispersed phase flux** (the default condition for walls)
- **Symmetry**

For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.

Mixture Properties

The **Mixture Properties** node contains the material properties for the continuous phase and the dispersed phase. It also contains settings for the viscosity model. For the Mixture Model, Turbulent Flow interfaces, the **Mixture Properties** node also adds the equations for the turbulence transport equations.

MODEL INPUTS

The viscosity of each phase can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a

locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The default **Absolute pressure** p_A is $p + p_{\mathrm{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIALS

Select the fluid materials to use for the material properties. The default material used for the **Continuous phase** is the **Domain material**. This corresponds to the material currently applied to the domain in question. The **Dispersed phase** uses **None** per default. A valid material must be selected instead.

CONTINUOUS PHASE PROPERTIES

The default **Density, continuous phase** ρ_c (SI unit: $\mathrm{kg/m^3}$) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case the default is 0 $\mathrm{kg/m^3}$.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref}, which are specified at the physics interface level.

The default **Dynamic viscosity, continuous phase** μ_c (SI unit: Pa·s), uses values **From material**. It describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. For **User defined** enter another value or expression. In this case, the default is 0 Pa·s.

DISPERSED PHASE PROPERTIES

The default **Density, dispersed phase** ρ_d (SI unit: kg/m^3) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case, the default is 0 kg/m^3.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref}, which are specified at the physics interface level.

Enter the **Diameter of particles/droplets** d_d (SI unit: m). The default is 10^{-3} m (1 mm). If **Haider-Levenspiel** is selected for the **Slip model** under **Physical Model**, enter a value between 0 and 1 for the **Sphericity** (dimensionless). The default is 1.

If **Liquid droplets/bubbles** is selected from the **Dispersed phase** list in the interface, then **Dynamic viscosity, dispersed phase** μ_d (SI unit: Pa·s) is also available. The default uses values **From material** (as selected in the **Materials** section) or select **User defined** to enter another value or expression. In this case, the default is 0 Pa·s.

MIXTURE MODEL

The options in this section are based on the selection made from the **Dispersed phase** list for the Mixture Model interfaces.

Slip Velocity Field

When a **User defined Slip model** is selected for the physics interface, specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data.

- When **Slip velocity** is set to **Specify slip velocity field**, enter the slip velocity between the two phases, $\mathbf{u}_{slip}$ (SI unit: m/s).
- When **Slip velocity** is set to **Specify slip flux**, enter the slip flux $\mathbf{j}_{slip}$ (SI unit: m/s).

- The Mixture Model Equations in Theory for the Mixture Model Interfaces

Mixture Viscosity Model

Select the **Mixture viscosity model**.

- When **Solid particles** is the **Dispersed phase**, select either **Krieger type** (the default) or **User defined**.
- When **Liquid droplets/bubbles** is the **Dispersed phase**, select **Krieger type** (the default), **User defined**, or **Volume averaged**.

For **User defined** enter a value or expression for the **Dynamic viscosity** μ (SI unit: Pa·s). The default is 0 Pa·s. When using this option, make sure to limit the viscosity to bounded positive values.

When **Krieger type** is selected, enter a value or expression for the **Maximum packing concentration** ϕ_{max} (dimensionless). The default is 0.62.

Select Krieger type to model the most generally valid expression for the mixture viscosity:

$$\mu = \mu_c\left(1-\frac{\phi_d}{\phi_{max}}\right)^{-2,5\phi_{max}\mu^*}$$

where ϕ_{max} is the maximum packing concentration, which for solid particles is approximately 0.62. The dimensionless parameter $\mu^* = 1$ for solid particles and

$$\mu^* = \frac{\mu_d + 0,4\mu_c}{\mu_d + \mu_c}$$

for droplets and bubbles. When applying the Krieger type viscosity model, ϕ_d is replaced by $\min(\phi_d, 0.999\phi_{max})$ for better robustness.

Select **Volume averaged** to model the mixture viscosity of liquid-liquid mixtures, which uses the following equation for the viscosity:

$$\mu = \phi_d \mu_d + \phi_c \mu_c$$

The Mixture Model interfaces always employ the mixture viscosity in the particle Reynolds number expression used to calculate the slip velocity, thereby accounting for the increase in viscous drag due to particle-particle interactions.

MIXING LENGTH LIMIT

This section is available for The Mixture Model, k-ε Interface, The Mixture Model, Realizable k-ε Interface, and The Mixture Model, k-ω Interface, where an upper limit on the mixing length is required.

When the **Mixing length limit** $l_{\text{mix,lim}}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression. The default is 1 (that is, one unit length of the model unit system).

DISTANCE EQUATION

This section is available for The Mixture Model, Algebraic yPlus Interface, The Mixture Model, L-VEL Interface, The Mixture Model, SST Interface, The Mixture Model, Low Re k-ε Interface, The Mixture Model, Spalart–Allmaras Interface, and The Mixture Model, v2-f Interface.

When the **Reference length scale** l_{ref} is set to **Automatic**, it is evaluated one tenth of the shortest side of the geometry bounding box. The solution to the wall distance equation is controlled by the parameter l_{ref}. The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling because small objects would have too large an impact on the solution if the wall distance were measured exactly. The automatic value is usually a good choice but the value can become too high if the geometry consists of several slim entities. In such cases, it is recommended that the reference length scale is defined manually. Select **Manual** to enter a different value or expression.

Mass Transfer

Use the **Mass Transfer** node to include mass transfer from the dispersed phase to the continuous phase.

MASS TRANSFER

Select a **Mass transfer model** — **User defined** (the default), **Nonequilibrium model**, or **Two-film theory**. For **User defined** enter a value or expression for the **Mass transfer from dispersed to continuous phase** m_{dc} (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

Nonequilibrium Model

For **Nonequilibrium model** enter values or expressions for each of the following:

- **Equilibrium volume fraction in dispersed phase** ϕ_{eq}. The default is 0.
- **Inverse time scales** f_c and f_d (SI unit: 1/s). The default is 0 s^{-1}.

The mass transfer is modeled as

$$m_{dc} = \rho_d[\max(f_c(\phi_d - \phi_{eq}), 0) - \max(f_d(\phi_{eq} - \phi_d), 0)]$$

Two-Film Theory

For **Two-film theory** enter values or expressions for each of the following:

- **Mass transfer coefficient** k (SI unit: m/s). The default is 0 m/s.
- **Species concentration in dispersed phase** c_d (SI unit: mol/m^3). The default is 0 mol/m^3.
- **Species concentration in continuous phase** c_c (SI unit: mol/m^3). The default is 0 mol/m^3.
- **Molecular weight of species** M (SI unit: kg/mol). The default is 0 kg/mol.

The mass transfer is modeled as

$$m_{dc} = k(c_d - c_c)Ma$$

where k denotes the mass transfer rate, and c_d and c_c are the species concentrations in the dispersed and the continuous phase, respectively. M is the species' molecular weight, and a is the interfacial area per unit volume between the two phases. The **Mass transfer model** — **Two-film theory** is available when the **Solve for interfacial area** checkbox is selected (under the **Physical Model** section).

Gravity

The **Gravity** node adds the force $\rho\mathbf{g}$ to the right-hand side of the momentum transport equation.

GRAVITY

Enter the components of the **Gravity vector**, $\mathbf{g}$ (SI unit: $\mathrm{m/s^2}$). The default value is (`0,-g_const`) where `g_const` is a physical constant equal to 9.8066 $\mathrm{m/s^2}$.

	For 2D components, gravity acts in the negative y direction by default. For example, in a 2D component, the y-component is `-g_const` and the other component is 0. In this setting, `g_const` is a predefined physical constant for the standard gravity (acceleration due to gravity at sea level).

	For 3D and 2D axisymmetric components, gravity acts in the negative z direction by default. For example, in a 3D component, the z-component is `-g_const` and the other components are 0. In this setting, `g_const` is a predefined physical constant for the standard gravity (acceleration due to gravity at sea level).

Initial Values

The **Initial Values** node adds initial values for the mixture velocity, pressure, and volume fraction of the dispersed phase, that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter values or expressions for the following dependent variables:

- **Velocity field, mixture**, the components of $\mathbf{j}$ (SI unit: m/s). The defaults are 0 m/s.
- **Pressure** p (SI unit: Pa). The default is 0 Pa.
- **Volume fraction, dispersed phase** (dimensionless). The default is 0.

- If the **Solve for interfacial area** checkbox is selected for the physics interface, enter an initial value for the **Number density, dispersed phase** nd (SI unit: $1/m^3$). The default is 0 $1/m^3$.
- If a **Schiller-Naumann** or a **Haider-Levenspiel** slip model is used in the physics interface, enter an initial value for the **Squared slip velocity** slipvel (SI unit: m^2/s^2). The default is 0.081 m^2/s^2.

For the Mixture Model, Turbulent Flow interfaces, initial values for the turbulence variables should be also specified. Additional initial values may be required for:

- **Turbulent kinetic energy** k
- **Turbulent dissipation rate** ep
- **Reciprocal wall distance** G
- **Specific dissipation rate** om
- **Undamped turbulent kinematic viscosity** υ_0
- **Wall distance in viscous units** yPlus
- **Tangential velocity in viscous units** uPlus
- **Turbulent relative fluctuations** zeta
- **Elliptic blending function** alpha

!	The following sections describe the available boundary conditions for the mixture and the dispersed phase volume fraction. In all equations, **n** denotes the outward pointing unit vector normal to the boundary.

Wall

The **Wall** node has boundary conditions available that describe the existence of a solid wall.

MIXTURE BOUNDARY CONDITION

Select a **Mixture boundary condition** for the wall.

- No Slip
- Slip
- Navier Slip

No Slip

No slip is the default boundary condition for the liquid. A no slip wall is a wall where the mixture velocity relative to the wall velocity is zero. For stationary walls, it sets the mixture velocity to zero at the wall:

$$\mathbf{j} = 0$$

For turbulent flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall functions** are selected, the **Apply wall roughness** option becomes available. Click to select the **Apply wall roughness** checkbox to apply the roughness correction. When the checkbox is selected, the default **Roughness model** is **Sand roughness**, which is derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

- For **Sand roughness** enter an **Equivalent sand roughness height** k_{seq} (SI unit: m). The default is 3.2 micrometers.
- For **Generic roughness** enter a **Roughness height** k_{s} (SI unit: m). The default is 3.2 micrometers. Then enter a **Roughness parameters** C_{s} (dimensionless). The default is 0.26.

References for the Single-Phase Flow, Turbulent Flow Interfaces

Slip

Select **Slip** to set the velocity component normal to the wall to zero $\mathbf{j} \cdot \mathbf{n}_{\text{wall}} = 0$.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{j} \cdot \mathbf{n}_{\text{wall}} = 0$, and adds a friction force of the form

$$\mathbf{F}_{\text{fr}} = -\frac{\mu}{\beta}\mathbf{j}_{\text{tang}}$$

where β is a slip length, and $\mathbf{j}_{\text{tang}} = \mathbf{j} - (\mathbf{j} \cdot \mathbf{n}_{\text{wall}})\mathbf{n}_{\text{wall}}$ is the velocity tangential to the wall. The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance β outside of the wall. In cases where the wall movement is nonzero, select the **Account for the translational wall velocity in the friction force** checkbox to use $\mathbf{j} - \mathbf{u}_{\text{bnd}} - ((\mathbf{j} -$

$\mathbf{u}_{bnd}) \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ instead of $\mathbf{j}_{tang}$ in the friction force. Then, the extrapolated tangential velocity component is $\mathbf{u}_{bnd}$ at a distance β outside of the wall. Note that the **Velocity of sliding wall** $\mathbf{u}_w$ is always accounted for in the friction force.

The Navier Slip boundary condition is suitable for walls adjacent to a free surface when solving for laminar flow. Applying this boundary condition, the contact line (fluid-fluid-solid interface) is free to move along the wall. Note that in problems with contact lines, the tangential velocity of the wall typically represents the movement of the contact line but the physical wall is not moving. In such cases, **Account for the translational wall velocity in the friction force** should not be selected.

The **Slip length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input. Select **User defined** from the **Slip length** list to manually prescribe β.

The Navier Slip option is not available when selecting a turbulence model.

DISPERSED PHASE BOUNDARY CONDITION

Select a **Dispersed phase boundary condition** — **No dispersed phase flux** (the default), **Dispersed phase concentration**, **Dispersed phase outlet**, **Dispersed phase flux**, or **Symmetry**.

- For **Dispersed phase concentration** enter a **Dispersed phase volume fraction** ϕ_{d0} (dimensionless). The default is 0. When **Solve for interfacial area** is selected under the **Physical Model** section, click either the **Dispersed phase number density** n_0 (SI unit: $1/m^3$) or **Diameter of particles/droplets** d_d (SI unit: m) button and enter a value or expression for n_0 (the default is $5 \cdot 10^6$ $1/m^3$) or d_d (the default is 1 mm).
- For **Dispersed phase flux** enter values or expression for the **Dispersed phase flux** $N_{\phi d}$ (SI unit: m/s) and, if **Solve for interfacial area** is selected under the **Physical Model** section, the **Number density flux** N_n (SI unit: $1/(m^2 \cdot s)$). The defaults are 0 m/s and 0 $1/(m^2 \cdot s)$, respectively.

Dispersed Phase Boundary Condition Equations

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{\mathbf{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{\mathbf{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u}_{\mathbf{tr}}$ becomes equal to the frame movement. $\mathbf{u}_{\mathbf{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u}_{\mathbf{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall** $\mathbf{u}_w$ should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.
- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.
- For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the **Velocity of moving wall, φ-component** v_w can also be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options.**

	Wall in the Single-Phase Flow interfaces

Inlet

The **Inlet** node adds a set of boundary conditions that describe inlets in fluid-flow simulations.

MIXTURE BOUNDARY CONDITION

Select a **Mixture boundary condition** for the inlet — **Velocity** (the default) or **Pressure**.

VELOCITY

For **Velocity** click the **Normal inflow velocity** (the default) or **Velocity field** buttons.

- For **Normal inflow velocity** enter a value or expression for J_0 (SI unit: m/s).
- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{j}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{j} = \mathbf{j}_0$$

PRESSURE

This condition specifies the normal stress which in most cases is approximately equal to the pressure. Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.

- The **Suppress backflow** checkbox is selected by default. This option adjusts the inlet pressure, $\hat{p}_0 \geq p_0$, locally in order to reduce the amount of fluid exiting the domain through the boundary. If suppress backflow is deselected, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.
- **Flow direction** controls in which direction the fluid enters the domain.
  - For **Normal flow** (the default) it prescribes zero tangential velocity component.
  - For **User defined** define an **Inflow velocity direction**, $\mathbf{d}_\mathbf{j}$ (dimensionless). The magnitude of $\mathbf{d}_\mathbf{j}$ does not matter, only the direction. $\mathbf{d}_\mathbf{j}$ must point into the domain.

DISPERSED PHASE BOUNDARY CONDITION

The default is **Dispersed phase concentration**. See Wall>Dispersed Phase Boundary Condition for the settings.

See Dispersed Phase Boundary Condition Equations for more information.

TURBULENCE CONDITIONS

This section is available for Mixture Model, Turbulent Flow interfaces so that the inlet conditions for the turbulence variables can be specified.

No additional inlet conditions are required for the algebraic turbulence models: Algebraic yPlus and L-VEL.

For the **Mixture Model, Spalart–Allmaras** interface, a value or expression for the **Undamped turbulent kinematic viscosity** υ_0 should be specified. The default value is `3*mm.nu`.

For transport-equation turbulence models, apart from Spalart–Allmaras, the following settings are available under the **Specify turbulence length scale and intensity** option:

- **Turbulent intensity** I_T
- **Turbulent length scale** L_T

For the v2-f turbulence model, the additional choice between **Isotropic turbulence** and **Specify turbulence anisotropy** appears. For **Specify turbulence anisotropy**, a value for the turbulent relative fluctuations at the inlet, ζ_0, may be specified. When **Specify turbulence variables** is selected, values or expressions for the dependent turbulence variables should be defined. Availability is based on the physics interface and the boundary condition chosen.

- **Turbulent kinetic energy** k_0
- **Turbulent dissipation rate** ε_0
- **Specific dissipation rate** ω_0
- **Turbulent relative fluctuations** ζ_0
- **Elliptic blending function** α_0

The turbulent length scale L_T and turbulence intensity I_T are related to the turbulence variables, see Theory for the Turbulent Flow Interfaces.

See Inlet in the Single-Phase Flow interfaces

Outlet

The **Outlet** node adds a selection of boundary conditions that describe outlets in fluid-flow simulations; that is, the conditions at boundaries where the fluid exits the domain.

MIXTURE BOUNDARY CONDITION

Select a **Mixture boundary condition** for the outlet — **Pressure** (the default) or **Velocity**.

PRESSURE CONDITIONS

The **Pressure** condition specifies the normal stress which in most cases is approximately equal to the pressure. The tangential stress component is set to 0 $\mathrm{N/m^2}$.

- Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0.
- Select the **Normal flow** checkbox to change the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The **Suppress backflow** checkbox is selected by default. This option adjusts the outlet pressure in order to reduce the amount of fluid entering the domain through the boundary.

VELOCITY

For **Velocity** click the **Normal outflow velocity** (the default) or **Velocity field** buttons.

- For **Normal outflow velocity** enter a value or expression for J_0 (SI unit: m/s).
- For **Velocity field** specify that the velocity at the boundary is equal to a given $\mathbf{j}_0$ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{j} = \mathbf{j}_0$$

DISPERSED PHASE BOUNDARY CONDITION

The default is **Dispersed phase outlet**. See Wall>Dispersed Phase Boundary Condition for the settings.

When the **Dispersed phase boundary condition** is set to **Dispersed phase outlet**, the **Exterior dispersed phase condition(s)** section contains an input field for the **Dispersed phase volume fraction** on the downstream side of the outlet. If **Solve for interfacial area** is selected at the physics interface level, additional input fields appear for the **Dispersed phase number density** or the **Diameter of particles/droplets** on the downstream side of the outlet.

See Dispersed Phase Boundary Condition Equations for more information.

See Outlet in the Single-Phase Flow interfaces

Symmetry

The **Symmetry** node adds boundary conditions that describe symmetry boundaries in fluid-flow simulations. The boundary condition for symmetry boundaries prescribes no penetration and vanishing tangential stress:

$$\mathbf{j} \cdot \mathbf{n} = 0, \qquad \mathbf{t}^T((\rho_c + \rho_d - \rho)\mathbf{u}_{slip}\mathbf{j}_{slip}^T + \tau_{Gm})\mathbf{n} = 0$$

BOUNDARY SELECTION

A boundary condition for 2D axial symmetry is not required.

For the symmetry axis at $r = 0$, the program automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the z direction and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group. Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

PRESSURE DIFFERENCE

A value or expression should be specified for the **Pressure difference**, $p_{src} - p_{dst}$. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context

menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options**.

ORIENTATION OF SOURCE

For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Interior Wall

The **Interior Wall** node adds a wall boundary condition on interior boundaries. It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall node specifies no flux for the dispersed phase.

	Dispersed Phase Boundary Condition Equations

MIXTURE BOUNDARY CONDITION

Select a **Mixture boundary condition** — **No slip** (the default) or **Slip**.

No Slip

No slip is the default boundary condition for the mixture. A no slip wall is a wall where the mixture velocity relative to the wall velocity is zero. For an interior stationary wall, it sets the mixture velocity to zero at the wall:

$$\mathbf{j} = 0$$

For turbulent flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall functions** are selected, the **Apply wall roughness** option becomes available. Click to select the **Apply wall roughness** checkbox to apply the roughness correction. When the checkbox is selected, the default **Roughness model** is **Sand roughness**, which is

derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

- For **Sand roughness** enter an **Equivalent sand roughness height** k_{seq} (SI unit: m). The default is 3.2 micrometers.
- For **Generic roughness** enter a **Roughness height** k_s (SI unit: m). The default is 3.2 micrometers. Then enter a **Roughness parameters** C_s (dimensionless). The default is 0.26.

References for the Single-Phase Flow, Turbulent Flow Interfaces

Slip

Select **Slip** to set the velocity component normal to the wall to zero $\mathbf{j} \cdot \mathbf{n} = 0$.

Navier Slip

The **Navier slip** condition enforces no-penetration at the wall, $\mathbf{j} \cdot \mathbf{n} = 0$, and adds a friction force of the form

$$\mathbf{F}_{fr} = -\frac{\mu}{\beta}\mathbf{j}$$

where β is a slip length. For more information, see the **Navier Slip** option in the Wall feature.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the

associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button ( ) and selecting **Advanced Physics Options.**

	Wall

Mixture Continuity

The **Mixture Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the Wall node is used as fallback unless another feature has been selected for the boundary.

	About Pairs

The Euler–Euler Model Interfaces

In this section:

- The Euler–Euler Model, Laminar Flow Interface
- The Euler–Euler Model, Turbulent Flow Interface
- Domain, Boundary, Point, and Pair Nodes for the Euler–Euler Model Interfaces

The Euler–Euler Model, Laminar Flow Interface

The **Euler-Euler Model, Laminar Flow (ee)** interface (), found under the **Multiphase Flow** > **Euler-Euler Model** branch () when adding a physics interface, can be used to simulate the flow of two continuous and fully interpenetrating incompressible phases (see Ref. 1 under the Theory for the Euler–Euler Model Interfaces). The physics interface can model flow at low and moderate Reynolds numbers. Typical applications are fluidized beds (solid particles in gas), sedimentation (solid particles in liquid), or transport of liquid droplets or bubbles in a liquid.

The physics interface solves two sets of Navier–Stokes equations, one for each phase, in order to calculate the velocity field for each phase. The phases interchange momentum as described by a drag model. The pressure is calculated from a mixture-averaged continuity equation and the volume fraction of the dispersed phase is tracked with a transport equation.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Phase Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Euler-Euler Model, Laminar Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is ee.

DISPERSED PHASE

Select a **Dispersed phase** — **Solid particles** or **Liquid droplets/bubbles**.

When **Solid particles** is selected, the Solid Pressure section is available in the Phase Properties node. Also see Dispersed Phase in the theory section.

PHYSICAL MODEL

Dispersed Phase

Select a **Dispersed phase** — **Solid particles** or **Liquid droplets/bubbles**.

When **Solid particles** is selected, the Solid Pressure section is available in the Phase Properties node. Also see Dispersed Phase in the theory section.

Reference Values

Reference values are global quantities used to evaluate the density of the fluid and define the absolute pressure.

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{\text{ref}}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the density of incompressible fluids.

Reference temperature The reference temperature is used to define the reference density.

TURBULENCE

Turbulence Model Type

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS, k-ε** (Reynolds-Averaged Navier–Stokes, k-ε).

DEPENDENT VARIABLES

The dependent variables (field variables) are:

- **Velocity field, continuous phase uc**
- **Velocity field, dispersed phase ud**
- **Pressure** p
- **Volume fraction, dispersed phase** phid

The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

Inconsistent stabilization can be activated independently for the momentum equation for the continuous phase, the momentum equation for the dispersed phase, and for the dispersed phase transport equation respectively by selecting the corresponding checkbox. Each inconsistent stabilization contribution has a tuning parameter.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

The **Residue volume fraction, continuous phase**, $\phi_{c,res}$, and **Residue volume fraction, dispersed phase**, $\phi_{d,res}$, set the smallest values used to avoid division by zero when evaluating terms that involve $1/\phi_c$ and $1/\phi_d$. Observe that this value does not prevent ϕ_c or ϕ_d from becoming smaller than $\phi_{c,res}$ and $\phi_{d,res}$, respectively.

Select the **Use pseudo time stepping for stationary equation form** checkbox to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable `CFLCMP` which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** CFL_{loc} (dimensionless).

DISCRETIZATION

The Euler-Euler Model, Laminar Flow interface supports three options for the basis functions: **P1+P1** (the default option), **P2+P1**, and **P3+P2**. They all represent Lagrangian basis functions of different orders:

- **P1+P1** – Linear basis functions for all degrees of freedom. Linear basis functions are computationally less expensive than the higher-order options and are also more

robust. This option requires that **Streamline diffusion** is activated for both of the momentum equations.

- **P2+P1** – Quadratic basis functions for all degrees of freedom except the pressure which is described by linear basis functions. Higher order elements, as compared to linear elements, are a computationally effective way to obtain high accuracy but only if the flow is well resolved. This requirement is most likely fulfilled for flows with very low velocities and/or small length scales.
- **P3+P2** – Cubic basis functions for all degrees of freedom except the pressure which is described by quadratic basis functions. This option is computationally very expensive and the least robust one but it is also the option with the highest formal accuracy.

To see all settings available in this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Isotropic Diffusion in the *COMSOL Multiphysics Reference Manual*
- Domain, Boundary, Point, and Pair Nodes for the Euler–Euler Model Interfaces
- Theory for the Euler–Euler Model Interfaces

The Euler–Euler Model, Turbulent Flow Interface

The **Euler–Euler Model, Turbulent Flow (ee)** interface ( ), found under the **Multiphase Flow** > **Euler–Euler Model** branch ( ) when adding a physics interface, can be used to simulate high Reynolds number flow of a two-phase mixture containing a continuous and a dispersed phase. The Euler–Euler model assumes that both phases are continuous, fully interpenetrating, and incompressible (see Theory for the Euler–Euler Model Interfaces). Typical applications for the interface are fluidized beds (solid particles in gas), sedimentation (solid particles in liquid), or transport of liquid droplets or bubbles in a liquid.

The physics interface solves two sets of Navier–Stokes equations, one for each phase, in order to calculate the velocity field for each phase. The phases interchange momentum as described by a drag model. The pressure is calculated from a mixture-

averaged continuity equation and the volume fraction of the dispersed phase is tracked with a transport equation.

Two-phase turbulence is modeled using the standard two-equation k-ε model with realizability constraints. The interface includes the possibility to solve one set of k-ε equations for the two-phase mixture, or to solve two sets of k-ε equations, one for each phase. Flow close to walls is modeled using wall functions.

Except where indicated below, the settings for this physics interface are the same as for The Euler–Euler Model, Laminar Flow Interface.

TURBULENCE

Turbulence Model Type

The default **Turbulence model type** is **RANS, k-ε**.

Two-Phase Turbulence

By default the **Two-Phase Turbulence** is defined as **Mixture**. This implies that one set of k-ε equations are solved for. To instead solve for two sets of k-ε equations, one for each fluid phase, select **Phase specific** (see Turbulent Two-Phase Flow Modeling).

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Turbulent Two-Phase Flow Modeling.

DEPENDENT VARIABLES

The following dependent variables (field variables) are defined for this interface:

- **Velocity field, continuous phase** u_c
- **Velocity field, dispersed phase** u_d
- **Pressure** p
- **Turbulent kinetic energy, mixture** k
- **Turbulent dissipation rate, mixture** ep
- **Turbulent kinetic energy, continuous phase** kc
- **Turbulent dissipation rate, continuous phase** epc
- **Turbulent kinetic energy, dispersed phase** kd
- **Turbulent dissipation rate, dispersed phase** epd

The names can be changed but the names of fields and dependent variables must be unique within a component.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**. The **Turbulence variables scale parameters** subsection is available when the **Turbulence model type** is set to **RANS, k-ε**.

In addition to the settings described for the Laminar Flow interface, enter a value for U_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The U_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units, or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver.

Domain, Boundary, Point, and Pair Nodes for the Euler–Euler Model Interfaces

The Euler–Euler Model Interfaces have the following domain, boundary, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- Flow Continuity
- Gravity
- Initial Values
- Inlet
- Interior Wall
- Mass Transfer
- Outlet
- Phase Properties
- Volume Force
- Wall

The following nodes are described for the Laminar Flow interface:

- Pressure Point Constraint

- Symmetry

!	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Phase Properties

The **Phase Properties** node has the material properties settings for the pure continuous and dispersed phases. It also has settings for the viscosity models for each of the two interpenetrating phases and the drag model. When the dispersed phase consists of solid particles, it also has settings for the solid pressure model.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The default **Absolute pressure** p_A is $p + p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MATERIALS

Select the materials to use for the material properties of the continuous phase and the dispersed phase respectively (when they are defined to take their values **From material**). By default, the default material used for the **Continuous phase** is the **Domain material**. This corresponds to the material currently applied to the domain in question. The **Dispersed phase** uses **None** per default. A valid material must be selected instead.

Other materials present can be selected from the **Continuous phase** or **Dispersed phase** list in order to use that material's properties for the liquid or gas, respectively.

CONTINUOUS PHASE PROPERTIES

Density, Continuous Phase

The default **Density, continuous phase** ρ_c (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression.

Dynamic Viscosity, Pure Continuous Phase

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. The dynamic viscosity of the pure continuous phase refers to the viscosity the fluid would have in the absence of the dispersed phase.

The default **Dynamic viscosity, pure continuous phase** μ_c (SI unit: Pa·s) uses values **From material**. The value of the viscosity is then the value defined for the material selected in the **Materials** section for the continuous phase. For **User defined** define a different value or expression.

DISPERSED PHASE PROPERTIES

The default **Density, dispersed phase** ρ_d (SI unit: kg/m^3) uses values **From material**. For **User defined** enter another value or expression.

Enter a value or expression for the **Diameter of particles/droplets** d_d (SI unit: m). The default is 10^{-3} m (1 mm).

The **Dynamic viscosity, pure dispersed phase** μ_d (SI unit: Pa·s) field is available when **Liquid droplets/bubbles** is selected as the **Dispersed phase** in The Euler–Euler Model Interfaces.

The default uses values **From material**. The value of the viscosity is then the value defined for the material selected in the **Materials** section for the dispersed phase. For **User defined** define a different value or expression.

VISCOSITY MODEL

Select a model for the **Mixture viscosity** — **Krieger type** (the default), **Volume average** (available for liquid droplets and bubbles) or **User defined**. Krieger type is appropriate for dispersed phases that do not form any pure phase regions. Volume average is more appropriate when the dispersed phase effectively can become the only phase in some regions.

- For **Krieger type**, select an option for **Maximum packing concentration**. The default is to use $\phi_{d,max} = 1.0$ for droplets and bubbles and $\phi_{d,max} = 0.62$ for particles. Select **User defined** to enter another value or expression for $\phi_{d,max}$.
- For **User defined** enter a value or expression for the **Mixture viscosity**. The default expression corresponds to the Krieger type viscosity with maximum packing equal to 0.62.

Select a **Dynamic viscosity model, continuous phase** — **Mixture viscosity** (default), **Pure phase value** or **User defined**. The **Mixture viscosity** option is appropriate when the maximum packing is controlled by the mixture viscosity. The **Pure phase value** option is more appropriate if the maximum packing is controlled in some other way, for example by solid pressure. Select **User defined** to enter an expression for the **Dynamic viscosity model, continuous phase**.

Select a **Dynamic viscosity model, dispersed phase** — **Mixture viscosity** (default), **Pure phase value** (available for bubbles and droplets), **Gidaspow** (available for solid particles) or **User defined**. The **Gidaspow** model prescribes $\mu_d^m = 0.5\phi_d$, which basically prescribes a small value for μ_d^m and should be combined with a solid pressure model.

DRAG MODEL

The models are described in The Euler–Euler Model Equations. When the dispersed phase corresponds to **Solid particles**, the **Schiller–Naumann**, **Hadamard–Rybczynzki, Ishii–Zuber**, **Gidaspow**, and **Haider–Levenspiel** models are available. For **Liquid droplets/bubbles**, the **Schiller–Naumann**, **Hadamard–Rybczynzki, Ishii–Zuber**, and **Tomiyama et al.** models are available. Select the **User-defined drag coefficient** option to specify an expression for the drag coefficient C_D.

- The **Schiller–Naumann** is valid for dispersed, rigid spheres and can be used for particle Reynolds numbers less than approximately $2.5 \cdot 10^5$. The Schiller–Naumann model is a general purpose model for diluted flows.
- The **Hadamard–Rybczynzki** is appropriate for diluted flows at low Reynolds numbers.
- The **Ishii–Zuber** model can for solid particles be regarded as a generalization of the Schiller–Naumann model in that it can be used also for dense flows. For droplets and bubbles, the Ishii–Zuber model also takes deformation of the fluid particles into account. The deformation depends on the **Surface tension coefficient**, σ. Use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**. Then select an option from the list that displays below (for example, **Water/Air**, **Glycerol/Air** and so forth). For **User defined** enter a value or expression for the surface tension coefficient σ (SI unit: N/m).
- The **Gidaspow** model describes the drag force coefficient for dispersed phase flows for all concentrations of the dispersed solid, including high concentrations.
- The **Haider-Levenspiel** model describes nonspherical particles for low and moderate particle Reynolds numbers. Enter a value between 0 and 1 for the **Sphericity** S_p (dimensionless).
- The **Tomiyama et al.** model describes the drag for diluted droplets and bubbles for any particle Reynolds number. The correlation is available in three versions, **Pure fluid**, **Slightly contaminated fluid** and **Contaminated fluid**. The Tomiyama *et al.* model depends on the **Surface tension coefficient**, σ that is selected in the same way as for the Ishii–Zuber model.

SOLID PRESSURE MODEL

The solid pressure models the particle dispersion due to collisions and friction between the solid particles. Details of the implemented models are described in Solid Pressure.

This section is available when **Solid particles** is selected as the **Dispersed phase** in The Euler–Euler Model Interfaces. Select a **Solid pressure model** ∇p_s.

- The **No solid pressure** (the default) disables solid pressure and leaves the collision to be described by a mixture viscosity. This option is appropriate for solid suspension, typically solids suspended in liquids.
- The other options, **Gidaspow-Ettehadieh**, **Gidaspow**, **Ettehadieh**, and **User-defined modulus of elasticity** describes particle-particle interaction for dispersed solids, typically solid particles in gas flows. These options should be combined with the Gidaspow model or a small user-defined value for μ_d^m.
- For **User-defined modulus of elasticity** enter an expression for the **Modulus of elasticity**, G (SI unit: N/m^2).

MIXING LENGTH LIMIT

When the **Mixing length limit** $l_{mix,lim}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression.

Initial Values

The **Initial Values** node adds initial values for the velocity fields for the continuous and dispersed phases, the pressure, and the volume fraction of the dispersed phase that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions in the tables for each component of:

- **Velocity field, continuous phase** uc
- **Velocity field, dispersed phase** ud

Enter initial values or expressions for:

- **Pressure** p
- **Volume fraction, dispersed phase** phid

For The Euler–Euler Model, Turbulent Flow Interface, initial values are needed for the turbulence variables. When **Mixture** is selected as **Two-phase turbulence**, enter values or expressions for:

- **Turbulent kinetic energy, mixture** k
- **Turbulent dissipation rate, mixture** ep

When **Phase specific** is selected as **Two-phase turbulence**, enter values or expressions for:

- **Turbulent kinetic energy, continuous phase** kc
- **Turbulent dissipation rate, continuous phase** epc
- **Turbulent kinetic energy, dispersed phase** kd
- **Turbulent dissipation rate, dispersed phase** epd

Mass Transfer

Use the **Mass Transfer** node to include mass transfer from the dispersed phase to the continuous phase.

MASS TRANSFER

Select a **Mass transfer model** — **User defined** (the default) or **Nonequilibrium model**. For **User defined** enter a value or expression for the **Mass transfer from dispersed to continuous phase** m_{dc} (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

Nonequilibrium Model

For **Nonequilibrium model** enter values or expressions for each of the following:

- **Equilibrium volume fraction in dispersed phase** ϕ_{eq}. The default is 0.
- **Inverse time scales** f_c and f_d (SI unit: 1/s). The default is 0 s^{-1}.

The mass transfer is modeled as

$$m_{dc} = \rho_d[\max(f_c(\phi_d - \phi_{eq}), 0) - \max(f_d(\phi_{eq} - \phi_d), 0)]$$

Interphase Velocity

Select **Dispersed phase velocity field** (the default) or **User defined**. For **User defined** enter a value or expression for each component of the interphase velocity $\mathbf{u}_{int}$.

Gravity

The **Gravity** node adds the gravity force vector to the right-hand side of the momentum equations; $\rho_c \mathbf{g}$ for the continuous phase and $\rho_d \mathbf{g}$ for the dispersed phase.

Gravity nodes are mutually exclusive, that is, there can only be one active Gravity node per domain.

GRAVITY

Enter the components of the **Gravity vector**, $\mathbf{g}$ (SI unit: m/s^2). For 2D components the default Gravity vector is defined as (0,-g_const). Here g_const is a physical constant equal to 9.8066 m/s^2. For 3D and 2D axisymmetric components, the gravity acts in the negative z direction by default.

Volume Force

The **Volume Force** node specifies the volume forces on the right-hand side of the momentum equations; $\mathbf{F}_c$ for the continuous phase and $\mathbf{F}_d$ for the dispersed phase. It may for example be used to add user defined interaction forces (in addition to the interphase drag force).

If several volume force nodes are added to the same domain, the sum of all contributions are added to the respective momentum equations.

Wall

The **Wall** node includes a set of boundary conditions to describe the flow conditions at a solid wall. The conditions for each phase are selected separately.

CONTINUOUS PHASE BOUNDARY CONDITION

Select a **Continuous Phase Condition** — **No slip** (the default), or **Slip**.

No Slip

A **No slip** condition models a wall where the velocity of the continuous phase relative to the wall velocity is zero. For a stationary wall, it sets the velocity of the continuous phase to zero:

$$\mathbf{u}_c = \mathbf{0}$$

For turbulent flows, wall functions are used to model the thin region near solid (no slip) walls with high gradients in the flow variables

Slip

The **Slip** option prescribes a no-penetration condition. For a stationary wall, $\mathbf{u}_c \cdot \mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops.

Leakage

Select the **Leakage** checkbox to specify an **Inward continuous phase mass flux**, $\dot{m}_c$ (SI unit: kg/(m^2·s)). This option is intended for small values of $\dot{m}_c$. For large mass fluxes, select an Inlet feature instead.

DISPERSED PHASE BOUNDARY CONDITION

Select a **Dispersed velocity boundary condition** — **No slip** (the default), or **Slip**. The conditions prescribed for the velocity of the dispersed phase correspond to those described for the continuous phase above.

Dispersed Phase Boundary Condition

The **Dispersed Phase Boundary Condition** defines the condition at the wall for the volume fraction of the dispersed phase.

- **No dispersed phase flux** prescribes a zero flux condition at the wall.
- Select **Leakage** to prescribe an **Inward dispersed phase mass flux**, $\dot{m}_d$ (SI unit: kg/(m^2·s)). This option is intended for small values of $\dot{m}_d$. For large mass fluxes, select an Inlet feature instead.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{tr}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{tr} = \mathbf{0}$. If the frame moves, $\mathbf{u}_{tr}$ becomes equal to the frame movement. $\mathbf{u}_{tr}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u}_{tr}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall** $\mathbf{u}_w$ should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.
- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

- Wall in the Single-Phase Flow interfaces
- The Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Inlet

The **Inlet** node prescribes the flow and turbulence conditions (when applicable) at a boundary where one or both phases enter the adjacent domain.

TWO-PHASE INLET TYPE

Selecting **Mixture** as the **Two-Phase Inlet Type**, inlet conditions are prescribed for both phases. Selecting **Continuous phase** or **Dispersed phase**, inlet conditions are prescribed for the corresponding phase, while wall conditions are applied to the remaining phase.

CONTINUOUS PHASE

The options available in this section are based on the **Two-phase inlet type** selected.

When **Mixture** or **Continuous phase** is selected as the **Two-phase inlet type** the **Velocity field, continuous phase** $\mathbf{u}_{c0}$ is prescribed.

When **Dispersed phase** is selected as the **Two-phase inlet type**, the conditions applied to the continuous phase are **No slip** ($\mathbf{u}_c=\mathbf{0}$) or **Slip** ($\mathbf{u}_c\cdot\mathbf{n}=0$, and no viscous stresses in the tangential directions).

Using the Phase specific option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the continuous phase turbulence variables.

- **Specify turbulent length scale and intensity** defines the turbulence inlet conditions using the **Turbulent intensity** $I_{T,c}$ (dimensionless) and the **Turbulence length scale** $L_{T,c}$ (SI unit: m).
- **Specify turbulence variables** prescribes the **Turbulent kinetic energy** $k_{0,c}$ (SI unit: m^2/s^2) and the **Turbulent dissipation rate** $\varepsilon_{0,c}$ (SI unit: m^2/s^3) at the inlet.

DISPERSED PHASE

The options available in this section are based on the **Two-phase inlet type** selected.

When **Mixture** or **Dispersed phase** is selected as the **Two-phase inlet type**, the **Velocity field, dispersed phase** $\mathbf{u}_{d0}$.

The **Dispersed phase boundary condition** can be **Volume fraction**, **Mass flux**, or **No flux**.

- For **Volume fraction**, specify the **Dispersed phase volume fraction**, ϕ_{d0}, at the inlet. This option locks the value of ϕ_d, but the exact flux depends on the dispersed phase velocity, $\mathbf{u}_{d0}$.
- For **Mass flux**, prescribe describe the **Inward dispersed phase mass flux**, $\dot{m}_d$ (SI unit: $kg/(m^2\cdot s)$). This option prescribes the flux for the dispersed phase, but the resulting volume fraction at the inlet depends on the dispersed phase velocity, $\mathbf{u}_{d0}$.

When **Continuous phase** is selected as the **Two-phase inlet type**, the conditions applied to the dispersed phase are **No slip** ($\mathbf{u}_d=\mathbf{0}$) or **Slip** ($\mathbf{u}_d\cdot\mathbf{n}=0$, and no viscous stresses in the tangential directions).

Using the Phase specific option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the dispersed phase turbulence variables.

- **Specify turbulent length scale and intensity** defines the turbulence inlet conditions using the **Turbulent intensity** $I_{T,d}$ (dimensionless) and the **Turbulence length scale** $L_{T,d}$ (SI unit: m).
- **Specify turbulence variables** prescribes the **Turbulent kinetic energy** $k_{0,d}$ (SI unit: m^2/s^2) and the **Turbulent dissipation rate** $\varepsilon_{0,d}$ (SI unit: m^2/s^3) at the inlet.

TURBULENCE CONDITIONS

Using the Mixture option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the mixture turbulence variables.

- **Specify turbulent length scale and intensity** defines the turbulence inlet conditions using the **Turbulent intensity** I_T (dimensionless) and the **Turbulence length scale** L_T (SI unit: m).
- **Specify turbulence variables** prescribes the **Turbulent kinetic energy** k_0 (SI unit: m^2/s^2) and the **Turbulent dissipation rate** ε_0 (SI unit: m^2/s^3) at the inlet.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

Outlet

This node is used to prescribe conditions at boundaries where the two-phase mixture exits the computational domain. The settings available in the node specifies conditions for the entire mixture, as opposed to the Inlet, Outlet and Wall nodes where the conditions for can be specified for each phase individually.

MIXTURE BOUNDARY CONDITION

Select **Mixture boundary conditions** — **Pressure, no viscous stress**, **Pressure**, **normal flow**, **Velocity**, **Degassing**, or **Filtration**.

Pressure Conditions

When **Pressure, no viscous stress** or **Pressure, normal flow** is selected as the **Mixture boundary condition**, specify the **Pressure** p_0 (SI unit: Pa) at the outlet. Note that the prescribed pressure should be consistent with the reference pressure level specified at the interface level as well as consistent with present volume forces (including gravity).

Velocity

Select **Velocity** to specify the **Velocity field, continuous phase** $\mathbf{u}_{c0}$ (SI unit: m/s) together with the **Velocity field, dispersed phase** $\mathbf{u}_d$ (SI unit: m/s) at the outlet.

Degassing and Filtration

Selecting **Degassing** allows the dispersed phase to exit the domain but prevents the continuous phase from exiting. This is achieved through a pressure (p_0), no viscous stress condition for the dispersed phase, in combination with a no penetration condition for the continuous phase.

Selecting **Filtration** on the other hand allows the continuous phase to exit the domain but prevents the dispersed phase from exiting. This is achieved through a pressure (p_0), no viscous stress condition for the continuous phase, in combination with a no penetration condition for the dispersed phase.

Pressure, no viscous stress is the least constraining option and allows the flow to exit the domain in nonnormal directions.

Pressure, normal flow restricts the flow to be completely normal to the outlet boundary. This option can influence the flow quite a bit upstream of the inlet.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-slip conditions on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed. It is compatible with laminar and turbulent flow. The conditions for each phase are selected separately.

CONTINUOUS PHASE BOUNDARY CONDITION

Select a **Continuous Phase Condition** — **No slip** (the default), or **Slip**.

No Slip

A **No slip** condition models a wall where the velocity of the continuous phase relative to the wall velocity is zero. For an interior stationary wall, it sets the velocity of the continuous phase to zero on both sides of the wall:

$$\mathbf{u}_c = \mathbf{0}$$

For turbulent flows, wall functions are used to model the thin region near solid walls with high gradients in the flow variables.

Slip

Slip prescribes a no-penetration condition. For a stationary interior wall, $\mathbf{u}_c \cdot \mathbf{n} = 0$ on both sides.

DISPERSED PHASE BOUNDARY CONDITION

Select a **Dispersed velocity boundary condition** — **No slip** (the default), or **Slip**. The conditions prescribed for the velocity of the dispersed phase correspond to those described for the continuous phase above.

Dispersed Phase Boundary Condition

The **Dispersed phase boundary condition** is set to **No dispersed phase flux**.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u}_{tr}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{tr} = \mathbf{0}$. If the frame moves, $\mathbf{u}_{tr}$ becomes equal to the frame movement. $\mathbf{u}_{tr}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u}_{tr}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**.

- Wall
- The Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the Wall node is used as fallback unless another feature has been selected for the boundary.

About Pairs

The Phase Transport Interfaces

In this section:

- The Phase Transport Interface
- The Phase Transport in Porous Media Interface
- The Phase Transport in Free and Porous Media Flow Interface
- Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces

The Phase Transport Interface

The **Phase Transport (phtr)** interface ( ), found under the **Fluid Flow** > **Multiphase Flow** > **Phase Transport** branch ( ), when adding a physics interface, is used to simulate the transport of multiple immiscible phases either in free flow or in flow through a porous medium. This interface solves for the averaged volume fractions (also called saturations in a porous medium) of the phases, and does not track the interfaces between the different phases, although microscopic interfacial effects are taken into account in the macroscopic equations for phase transport in porous media through the capillary pressure functions. The **Phase Transport** interface can be used for stationary and time-dependent analyses.

The main feature is the **Fluid** node, which provides an interface for defining the phase material along with the transporting flow properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click the **Phase Transport** node to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `phtr`.

PHASES

Select the volume fraction of the phase that this physics interface solves for using the volume constraint in equation Equation 6-3 (that is, its value comes from the fact that the sum of all volume fractions must equal 1). In the **From volume constraint** list, select the volume fraction of the preferred phase. By default, the first volume fraction is used:

$$s_1 = 1 - \sum_{i=2}^{N} s_i \tag{6-3}$$

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There are two consistent stabilization methods: **Streamline diffusion** and **Crosswind diffusion**. Both checkboxes for these methods are selected by default and should remain selected for optimal performance. Consistent stabilization methods do not perturb the original transport equation.

Select the **Use dynamic subgrid time scale** checkbox to estimate the influence of temporal variations in the velocity field, instead of using the inverse time step, in the consistent stabilization terms. This checkbox is selected by default

Select the **Limit small time steps effect on stabilization time scale** checkbox to prevent loss of stabilization at small time steps.

There is one inconsistent stabilization method: **Isotropic diffusion**. This method is equivalent to adding a diffusion term to the equations in order to dampen the effect of oscillations by making the system somewhat less dominated by convection. By default, the **Isotropic diffusion** checkbox is not selected because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. If required, select the **Isotropic diffusion** checkbox and enter a **Tuning parameter** as a scalar positive value. The default value is 0.25. A higher value adds more isotropic diffusion.

- Numerical Stability — Stabilization Techniques for Fluid Flow

GRAVITY EFFECTS

When the **Include gravity** checkbox is selected, a global **Gravity** feature is shown in the interface model tree, and the gravitational force is added to the phase transport equations in porous domains. For more information, see Gravity.

QUADRATURE SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

These settings affect the numerical integration, and you do not normally need to change them. The **Use automatic quadrature settings** checkbox is selected by default, meaning that the settings are taken from the main equation in the interface.

If the checkbox is cleared, the following setting become available:

Integration Order

The **Integration order** specifies the desired accuracy of integration during discretization. Polynomials of at most the given integration order are integrated without systematic errors. For smooth constraints, a sufficient integration order is typically twice the order of the shape function. For example, the default integration order for linear elements is 2. The integration order is a positive integer.

The settings in this section currently only affect the integration order in the **Fluid** and **Porous Medium** domain features.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Pseudo Time Stepping

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary** equation form is used in order to speed up convergence. When selected, a CFL number expression should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs-

Lewy condition) is determined by a PID regulator. The **Use pseudo time stepping for stationary equation form** option is enabled by default.

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Pseudo Time Stepping for Mass Transport

DISCRETIZATION

You can choose the order of the shape functions used for the volume fraction variables. The default shape functions are **Linear** Lagrange.

To display all settings available in this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

The **Value type when using splitting of complex variables** setting should in most pure mass transport problems be set to **Real** which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

Add or remove volume fractions of different phases in the model and also change the names of the dependent variables that represent the volume fractions.

Specify the **Number of phases**. There must be at least two phases. To add a single phase, click the **Add volume fraction** button (+) under the table. To remove a volume fraction, select it in the list and click the **Remove volume fraction** button ( ) under the table. Edit the names of the phases directly in the table.

The Phase Transport in Porous Media Interface

The **Phase Transport in Porous Media** interface ( ), found under the **Fluid Flow** > **Multiphase Flow** > **Phase Transport** branch ( ), is used to simulate the transport of multiple phases either in free flow or in flow through a porous medium. The interface is the same as the **Phase Transport** interface but it uses other defaults: a **Porous Medium** node is added by default, instead of a **Fluid** node.

This interface is dedicated to modeling transport of multiple immiscible phases in a porous medium, taking into account their relative permeabilities and capillary pressures.

The **Phase Transport in Porous Media** interface can be used for stationary and time-dependent analyses.

The main feature is the **Porous Medium** node, which provides an interface for defining the phase materials along with the transporting porous medium flow properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Porous Medium**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click the **Phase Transport in Porous Media** node to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as for the **Phase Transport** interface.

The Phase Transport in Free and Porous Media Flow Interface

The **Phase Transport in Free and Porous Media Flow** interface ( ), found under the **Fluid Flow** > **Multiphase Flow** > **Phase Transport** branch ( ), is used to simulate the transport of multiple phases both in free flow and in flow through a porous medium. The interface is the same as the **Phase Transport** interface but it uses other defaults: both a **Fluid** and a **Porous Medium** node are added by default. In addition a default **Free-Porous Interface** boundary condition is added.

The **Phase Transport in Free and Porous Media Flow** interface can be used for stationary and time-dependent analyses.

The main features are:

- The **Fluid** node, which provides a user interface for defining the phase material along with the transporting flow properties.
- The **Porous Medium** node, which provides a user interface for defining the phase materials along with the transporting porous medium flow properties.
- The **Free-Porous Interface** node, which provides a user interface for defining the interfacial condition applied at the free-porous interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Porous Medium**, **No Flux** (the default boundary condition), **Free-Porous Interface**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click the **Phase Transport in Free and Porous Media Flow** node to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as for the **Phase Transport** interface.

Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces

The **Phase Transport** and **Phase Transport in Porous Media** interfaces have the following domain, boundary, edge, and point nodes (listed in alphabetic order) available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- Continuity
- Boundary Mass Source
- Fluid
- Fluid (Porous Medium)
- Free-Porous Interface
- Gravity
- Initial Values
- Interior Wall
- Mass Flux
- Mass Source
- No Flux
- Open Boundary
- Outflow
- Periodic Condition
- Porous Matrix
- Porous Medium
- Porous Medium Discontinuity
- Turbulent Mixing
- Volume Fraction

Fluid

For this node, the Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu.

VELOCITY FIELD

Specify the velocity field for each phase that is not computed from the volume constraint. Select the source of the Velocity field. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a fluid flow interface added to the model component. These physics interfaces are available for selection in the velocity field list.

DENSITY

Enter the **Density** ρ (SI unit: $\mathrm{kg/m^3}$) of each phase. The default value is 1000 $\mathrm{kg/m^3}$.

Turbulent Mixing

This subnode is available from the context menu (right-click the Fluid parent node) as well as from the **Physics** toolbar, **Attributes** menu. Use this node to account for the turbulent mixing caused by the eddy diffusivity. An example is when the specified velocity field corresponds to a RANS solution.

TURBULENT MIXING PARAMETERS

Some physics interfaces provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** ν_T list. The list always contains the **User defined** option where any value or expression can be entered.

The default **Turbulent Schmidt number** $\mathrm{Sc_T}$ is 0.71 (dimensionless).

FURTHER READING

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

Porous Medium

Use this node to model the transport of multiple phases through a porous medium. Multiphase transport is affected by the properties of the different phases, as well as properties of the solid matrix. These properties are defined in the Fluid (Porous Medium) and Porous Matrix subnodes, respectively.

Fluid (Porous Medium)

Use this node to specify the properties of the different phases, including their relative permeabilities and capillary pressures.

MODEL INPUT

Enter the absolute pressure field (SI unit: Pa) for the phase that is computed from the volume constraint. The volumetric flux of this phase is computed using Darcy's law, and in many cases that pressure field will be computed for in a **Darcy's Law** interface, coupled to the **Phase Transport** interface using a **Multiphase Flow in Porous Media** multiphysics coupling node.

The volumetric fluxes of the other phases are also computed using Darcy's law, taking into account the relative permeabilities and capillary pressures.

CAPILLARY PRESSURE

Select a **Capillary pressure model** — **User defined** (the default), **van Genuchten**, **Brooks and Corey**, or **Capillary diffusion**. The **van Genuchten** and **Brooks and Corey** options are only available when there are not more than two phases present in the model.

- For **User defined**, enter an expression for the **Capillary pressure** p_c (SI unit: Pa) for the phases that are not computed from the volume constraint. The pressure of the corresponding phase is equal to the pressure of the phase computed from the volume constraint (supplied in the **Pressure** input field) plus the capillary pressure supplied for this phase.
- For **van Genuchten**, select the **Wetting phase** and enter an **Entry capillary pressure** p_{ec} (SI unit: Pa), the **Constitutive relations constant** m_{vG} (dimensionless), and **Constitutive relations constant** l_{vG} (dimensionless).
- For **Brooks and Corey**, select the **Wetting phase** and enter an **Entry capillary pressure** p_{ec} (SI unit: Pa) and the **Pore size distribution index** λ_p (dimensionless).
- For **Capillary diffusion**, enter a capillary diffusion coefficient D_c (SI unit: m^2/s) for the phases that are not computed from the volume constraint.

PHASE PROPERTIES

Select the material to use for each phase. Select **Domain material** (the default) from the **Fluid** list to use the material defined for the domain. Select another material to use that material's properties.

Enter the **Density** ρ (SI unit: kg/m^3), **Dynamic viscosity** μ (SI unit: Pa·s) and **Relative permeability** κ_r (a dimensionless number between 0 and 1) for each phase. The defaults for the **Density** and **Dynamic viscosity** are **From material**, and **User defined** for the **Relative permeability**. For **User defined**, the default values are 1000 kg/m^3, 0.001 Pa·s. and s_i^2, respectively.

The **Relative permeability** input fields are only available when the **Capillary pressure model** is set to **User defined** or **Capillary diffusion**. In these cases, select either **User defined** or **Power law**. When **Power law** is selected, enter the **Exponent** q_i (dimensionless, default value 2) and the **Residual saturation** s_{ri} (dimensionless, default value 0)

In the other cases (**van Genuchten** or **Brooks and Corey**) the relative permeabilities are defined by the **van Genuchten** or **Brooks and Corey** model. For the **van Genuchten** and **Brooks and Corey** model, specify the **Residual saturation** s_{ri} (dimensionless, default value 0) for each phase.

Porous Matrix

This node defines the porosity and permeability of the solid matrix of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** (the default) from the **Porous material** list to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From material**, defined by the **Porous material** selected. For **User defined** the default is 0.5.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material** selected. For **User defined** the default is the **Isotropic** scalar value of `1e-9` m^2. To define a tensor value, select **Diagonal**, **Symmetric**, or **Full**, and enter values or expressions in the matrix.

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Gravity Effects** settings. It defines the gravity forces from the **Gravity vector** value. Note that this feature only has an effect in porous domains.

GRAVITY

Enter the components of the **Gravity vector g**. The default value is `g_const` which is the physical constant having the value 9.8066 m/s^2.

- For 3D and 2D axisymmetric models, the default value is `-g_const` in the z direction.
- For 2D models, the default value is `-g_const` in the y direction.

Initial Values

The **Initial Values** node specifies the initial values for the volume fraction of each phase. These serve as an initial guess for a stationary solver or as initial condition for a transient simulation.

DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

INITIAL VALUES

Enter a value or expression in the field for the volume fraction of each phase except for the one computed from the volume constraint.

Mass Source

In order to account for consumption or production of the different phases due to one or more reactions or other physical processes, the **Mass Source** node adds source terms to the right-hand side of the phase transport equations.

MASS SOURCE

Add an expression for the mass source for each individual phase present, except for the one computed from the volume constraint. The net mass source of all phases together is assumed to be zero, which means that the mass is transferred to or from the phase that is computed from the volume constraint.

Select the **Mass transfer to other phases** checkbox if mass is transferred from or to phases not accounted for in the phase transport interface, for instance when mass is released or absorbed by the solid part of the porous matrix. In this case the mass source for the phase calculated from the volume constraint should also be specified. The net mass transfer corresponds to the sum of the mass sources for all phases and should be accounted for in the computation of the flow field. When the **Phase Transport in Porous Media** interface is coupled to a **Darcy's Law** interface using a **Multiphase Flow in Porous Media** multiphysics coupling node, this is done automatically.

Boundary Mass Source

In order to account for consumption or production of the different phases due to one or more reactions or other physical processes at a boundary, the **Boundary Mass Source** node adds mass flux terms at the selected boundaries.

BOUNDARY MASS SOURCE

Add an expression for the mass source for each individual phase present. The net mass transfer corresponds to the sum of the mass sources for all phases and should be accounted for in the computation of the flow field. When the **Phase Transport in Porous Media** interface is coupled to a **Darcy's Law** interface using a **Multiphase Flow in Porous Media** multiphysics coupling node, this is done automatically.

No Flux

This node is the default boundary condition on exterior boundaries. It represents boundaries where no mass flows in or out of the boundaries. Hence, the total flux is zero.

Volume Fraction

This node adds a boundary condition for the volume fractions of the different phases. Set the volume fractions of all phases except the one computed from the volume constraint. This ensures that the sum of the volume fractions is equal to one.

VOLUME FRACTION

Specify the volume fraction for each phase individually. Select the checkbox for the phases to specify the volume fraction, and enter a value or expression in the corresponding field. To use another boundary condition for a specific phase, click to clear the checkbox for the volume fraction of that phase.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

Mass Flux

Three different types of nodes are available to add a mass flux to the Phase Transport physics interface.

The **Mass Flux** node can be used to specify the total mass flux of a phase across a boundary. This node is available for surfaces in 3D geometries, edges in 2D and 2D axisymmetric geometries and points in 1D and 1D axisymmetric geometries.

For modeling mass flux from very thin objects add a **Line Mass Source** or a **Point Mass Source** node.

The **Line Mass Source** node adds mass flow originating from a tube of infinitely small radius. It is available for edges in 3D geometries or points in 2D and 2D axisymmetric geometries.

The **Point Mass Source** node models mass flow originating from an infinitely small sphere centered around a point. It is available for points in 3D geometries.

In all three types of nodes, set the mass flux for all phases except the one computed from the volume constraint. This ensures that the sum of the volume fractions is equal to one.

MASS FLUX

Specify the inward mass flux for each phase individually. Select the checkbox for the phase to prescribe a mass flux and enter a value or expression for the flux in the corresponding field. To use another boundary condition for a specific phase, click to clear the checkbox for the flux of that phase. Use a positive value for an inward flux. The units are based on the type of node: **Mass Flux** node: kg/(m^2·s), **Line Mass Source** node: kg/(m·s), and **Point Mass Source** node: kg/s.

Outflow

Set this condition at exterior boundaries where the phases are transported out of the model domain by fluid motion. The outward mass flux for each phase is in this case set to the normal outward phase velocity times the phase density.

Open Boundary

Use this node to set up transport across boundaries where both convective inflow and outflow occur. On the parts where fluid flows into the domain, an exterior species concentration is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Phase Transport interface.

The **Open Boundary** condition is only available for exterior boundaries adjacent to a **Phase Transport Properties** domain and thus it is not applicable for exterior boundaries adjacent to a porous domain.

EXTERIOR VOLUME FRACTION

Specify a value or expression for the **Exterior volume fraction** for each phase not computed from the volume constraint.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the volume fraction across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying a no-flux condition on interior curves and surfaces instead.

Porous Medium Discontinuity

The **Porous Medium Discontinuity** boundary condition can only be applied on interior boundaries, and only when on both sides of the boundary a **Porous Medium** domain condition is active. Set this condition at boundaries over which the capillary pressure function is discontinuous in the phase saturations due to the different properties of the porous matrix on both sides of the discontinuity.

POROUS MEDIUM DISCONTINUITY SETTINGS

This section is only available when only two phases are present in the physics interface. Select the checkbox to use automatic settings in this case.

ENTRY CAPILLARY PRESSURE

This section is only available if the automatic settings are not used for the **Porous Medium Discontinuity Settings**, or when the **Porous Medium Discontinuity Settings** section is not available, which is the case if there are three or more phases present.

Specify on which side of the discontinuity the lower permeable medium is located using the settings for the **Location of lower permeable medium**.

Specify the **Entry capillary pressure** p_{ec} (SI unit: Pa) for all phases, except the one computed from the volume constraint. Make sure the values correspond to the settings for the capillary pressure model in the adjacent domain conditions.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the volume fraction for each phase is continuous across the pair.

A No Flux subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **No Flux** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Continuity** node, additional fallback feature subnodes can be added.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. The **Constraints** settings can be set to **Use pointwise constraints** (default) or to **Use DG constraints (if possible)**. This latter option uses DG constraints as long as the selected boundaries are not adjacent to a porous domain. If the boundary selection contains boundaries adjacent to a porous domain, pointwise constraints are used instead. DG constraints are recommended on

pairs adjacent to a Fluid feature, especially when the mesh nodes do not match across the pair or when the mesh is sliding.

Depending on the constraint method selected, the following settings are available:

- **Apply reaction terms on** can be set to **Individual dependent variables** (default) or **All physics (symmetric)**. This setting is not available when **Use DG constraints** is selected.
- Select **Elemental** (default) or **Nodal** under **Constraint method**. This setting is available for **Use pointwise constraints**.

Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the phase transport between two sets of boundaries. The node prescribes continuity in the volume fractions and mass fluxes between the "source" and "destination" side respectively. Note that these names are arbitrary and do not influence the direction in which mass is transported. It is dictated by the phase transport equations in the adjacent domains.

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

For more complex geometries, it might be necessary to add the **Destination Selection** selection, with which you can specify the boundaries that constitute the destination surfaces.

BOUNDARY SELECTION

The software usually automatically identifies the boundaries as either source boundaries or destination boundaries, as indicated in the selection list. This works fine for cases like opposing parallel boundaries. In other cases, right-click **Periodic Condition** and select **Manual Destination Selection** to control the destination. By default it contains the selection that COMSOL Multiphysics identifies.

DESTINATION SELECTION

This section is available for specifying the destination boundaries, if needed, when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Condition** node. You can only select destination boundaries from the union of all source and destination boundaries.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. The **Constraints** settings can be set to **Use pointwise constraints** (default) or to **Use DG constraints (if possible)**. This latter option uses DG constraints as long as the selected boundaries are not adjacent to a porous domain. If the boundary selection contains boundaries adjacent to a porous domain, pointwise constraints are used instead. DG constraints are recommended on boundaries adjacent to a Fluid feature, especially when the mesh nodes do not match across the source and destination boundaries.

Depending on the constraint method selected, the following settings are available:

- **Apply reaction terms on** can be set to **Individual dependent variables** (default) or **All physics (symmetric)**. This setting is not available when **Use DG constraints (if possible)** is selected.
- Select **Elemental** (default) or **Nodal** under **Constraint method**. This setting is available for **Use pointwise constraints**.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping Between Source and Destination** section, see Mapping Between Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Free-Porous Interface

The **Free-Porous Interface** boundary condition can only be applied on interior boundaries, and only when on one sides of the boundary a **Fluid** domain condition and on the other side a **Porous Medium** domain condition is active. Apply this condition at boundaries where there is an interface between free flow and porous media flow.

PHASES

The number of **Phase** sections depends on the number of phases defined in the parent Phase Transport interface: the number of sections is equal to the number of phases not computed from the volume constraint, which is equal to the number of phases defined in the Phase Transport interface minus one.

Select the interfacial condition for each phase that is not computed from the volume constraint. The following options are available:

- **Residual saturation** sets the phase saturation on the porous side of the free-porous interface equal to the phase residual saturation, specified in the adjacent **Porous Medium** node. (Note that the residual saturation can only be specified if one of the predefined capillary pressure models is selected in the adjacent **Porous Medium** node. For user defined capillary pressure models, the residual saturation is taken to be equal to 0.)
- **Outflow, no flux below threshold saturation** sets a maximum threshold phase saturation for the phase saturation on the porous side of the free-porous interface and only allows the phase to flow out of the porous domain, while there will be no flux of the phase across the free-porous interface when the phase saturation is below the specified threshold saturation $s_{0,i}$.
- **Ratio of free flow volume fraction** specifies the ratio $r_{0,i}$ between the phase saturation on the porous side and the phase volume fraction on the free-flow side of the free-porous interface.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

The Phase Transport Mixture Model Interfaces

The Phase Transport Mixture Model, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the **Fluid Flow** > **Multiphase Flow** > **Phase Transport Mixture Model** branch of the **Model Wizard** or **Add Physics** windows, one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) and the **Phase Transport** interface are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Mixture Model**.

The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

- The **Laminar Flow** interface ( ) combines a Phase Transport interface with a Laminar Flow interface.
- The **Turbulent Flow, Algebraic yPlus** interface ( ) combines a Phase Transport interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface ( ) combines a Phase Transport interface with a Turbulent Flow, L-VEL interface.
- The **Turbulent Flow, k-ε** interface ( ) combines a Phase Transport interface with a Turbulent Flow, k-ε interface.
- The **Turbulent Flow, Realizable k-ε** interface ( ) combines a Phase Transport interface with a Turbulent Flow, Realizable k-ε interface.
- The **Turbulent Flow, k-ω** interface ( ) combines a Phase Transport interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, SST** interface ( ) combines a Phase Transport interface with a Turbulent Flow, SST interface.

- The **Turbulent Flow, Low Re k-ε** interface ( ) combines a Phase Transport interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, Spalart–Allmaras** interface ( ) combines a Phase Transport interface with a Turbulent Flow, Spalart–Allmaras interface.
- The **Turbulent Flow, v2-f** interface ( ) combines a Phase Transport interface with a Turbulent Flow, v2-f interface.

Coupling Feature

The Mixture Model multiphysics coupling node is described in this section.

Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

PHASE TRANSPORT

The available physics features for The Phase Transport Interface are listed in the section Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, ALGEBRAIC YPLUS

The available physics features for The Turbulent Flow, Algebraic yPlus Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, L-VEL

The available physics features for The Turbulent Flow, L-VEL Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ε

The available physics features for The Turbulent Flow, k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, REALIZABLE k-ε

The available physics features for The Turbulent Flow, Realizable k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ω

The available physics features for The Turbulent Flow, k-ω Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE k-ε

The available physics features for The Turbulent Flow, Low Re k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SPALART–ALLMARAS

The available physics features for The Turbulent Flow, Spalart–Allmaras Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, V2-F

The available physics features for The Turbulent Flow, v2-f Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

Mixture Model

Use the **Mixture Model** ( ) multiphysics coupling to simulate the flow of liquids containing one or more dispersed phases. The dispersed phases can be bubbles, liquid droplets, or solid particles, which are assumed to travel always with their terminal velocity.

The Phase Transport and the single-phase flow interface, which are coupled by the **Mixture Model** multiphysics coupling, solve together for conservation of mass of the dispersed phases and conservation of total mass and momentum of the mixture.

The **Mixture Model** multiphysics coupling provides the mixture density and viscosity to the single-phase fluid flow interface. Since the density of the mixture depends on the volume fractions and densities of the different phases, which in turn may depend on pressure and temperature, it cannot be assumed that the density of the mixture is constant. Therefore the **Incompressible flow** option is not available in the single-phase flow interface that is coupled by the **Mixture Model** multiphysics coupling.

In the Phase Transport interface, it sets the **Absolute pressure** in the **Model Input** section and defines the densities in the **Density** section of the **Fluid** feature. In addition it determines and provides the velocity fields for the dispersed phases in the **Velocity Field** section.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `mfmm1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the mixture model, or select **All domains** as needed.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Phase transport** and **Fluid flow** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Phase Transport** is deleted, then the **Phase transport** list defaults to **None** as there is nothing to couple to.

MODEL INPUTS

The viscosity and density of each phase can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **User defined**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The default **Absolute pressure** p_A is $p+p_{\text{ref}}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

Whenever the **Compressibility** in the coupled **Fluid flow** interface is set to **Weakly compressible flow**, the material properties are evaluated using the reference pressure level, p_{ref}, supplied in the coupled **Fluid flow** interface.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

PHYSICAL MODEL

Specify the characteristics of the dispersed phase(s), the model for the slip velocity, and the mixture viscosity model.

Dispersed Phase

To characterize the **Dispersed phase**, select **Solid particles** (the default) or **Liquid droplets/bubbles**.

Slip Model

To compute the slip velocity $\mathbf{u}_{\text{slip},i}$ (SI unit: m/s), select a **Slip model** — **Homogeneous flow** (the default), **Hadamard-Rybczynski**, **Schiller-Naumann**, **Haider-Levenspiel**, or **User defined**.

- The **Homogeneous flow** model assumes that the velocities of the continuous and dispersed phases are equal, that is, $\mathbf{u}_{\text{slip},i} = 0$.
- In most cases there is a significant difference in the velocity fields due to the buoyancy of the dispersed phase. Use one of the predefined slip models for such cases.
- For **User defined** specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data. Enter the **Slip velocity field** $\mathbf{u}_{\text{slip},i}$ (SI unit: m/s) in the Dispersed phase properties sections.

Mixture Viscosity Model

Select the **Mixture viscosity model**.

- When **Solid particles** is the **Dispersed phase**, select either **Krieger type** (the default) or **User defined**.
- When **Liquid droplets/bubbles** is the **Dispersed phase**, select **Krieger type** (the default), **Volume averaged**, or **User defined**.

For **User defined** enter a value or expression for the **Dynamic viscosity, mixture** μ (SI unit: Pa·s). The default expression is `mfmm1.muc`, which is the variable name for the viscosity of the continuous phase. When using this option to enter an expression, make sure to limit the viscosity to bounded positive values.

When **Krieger type** is selected, enter a value or expression for the **Maximum packing concentration** ϕ_{max} (dimensionless). The default is 0.62.

Select Krieger type to model the most generally valid expression for the mixture viscosity:

$$\mu = \mu_c\left(1 - \frac{\phi_d}{\phi_{max}}\right)^{-2,5\phi_{max}\mu^*}$$

where ϕ_{max} is the maximum packing concentration, which for solid particles is approximately 0.62. The dimensionless parameter $\mu^* = 1$ for solid particles and

$$\mu^* = \frac{\mu_d + 0,4\mu_c}{\mu_d + \mu_c}$$

for droplets and bubbles. When applying the Krieger type viscosity model, ϕ_d is replaced by $\min(\phi_d, 0.999\phi_{max})$ for better robustness.

When there is more than one dispersed phase, the Krieger type viscosity model uses a more involved expression which is described in detail in the section Theory for the Phase Transport Mixture Model Interfaces

Select **Volume averaged** to model the mixture viscosity of liquid-liquid mixtures, which uses the following equation for the viscosity:

$$\mu = \sum_{i=1}^{N} s_i \mu_i$$

The Mixture Model interfaces always employ the mixture viscosity in the particle Reynolds number expression used to calculate the slip velocity, thereby accounting for the increase in viscous drag due to particle-particle interactions.

Include Diffusion Stress in Momentum Equation

When the **Include diffusion stress in momentum equation** checkbox is selected (default), the diffusion stress term is added to the momentum equation in the coupled fluid flow interface. Deselect the checkbox to disregard this term.

Low Dispersed Phase Concentration

When the **Low dispersed phase concentration** checkbox is selected, the mixture density in the continuity equation and in the inertial terms of the momentum equation is replaced by the density of the continuous phase (see Equation 6-135 and Equation 6-136 in the section Theory for the Phase Transport Mixture Model Interfaces). This

approximation is valid if the volume fraction of the dispersed phases is small (less than a few percent) and if the density of the dispersed phases is not (much) larger than the density of the continuous phase.

Include Shear-Induced Migration

When the **Include shear-induced migration** checkbox is selected, shear-rate dependent diffusion and migration terms are added to the conservation equations for the volume fractions of the dispersed phases. Enter values for the parameters K_c and λ (the default values are 0.4 and 1.59, respectively).

TURBULENCE

This section is available whenever the coupled fluid flow interface is a turbulent flow interface using a RANS turbulence model.

Enter a value or expression for the **Turbulent Schmidt number** $\mathrm{Sc_T}$. The default value is 0.35 (dimensionless).

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

Whenever the coupled fluid flow interface is a turbulent flow interface using the k-ε, k-ω, SST, Low Re k-ε or Realizable k-ε turbulence model, and the **Dispersed phase** is set to **Liquid droplets/bubbles**, this section also contains an **Include bubble-induced turbulence** checkbox. When this checkbox is selected, bubble induced turbulence production terms are added to the turbulence model. In addition, the turbulence model parameters for these terms can be edited.

CONTINUOUS PHASE PROPERTIES

Select the fluid materials to use for the material properties. The default material used for the **Continuous phase** is the **Domain material**.

The default **Density, continuous phase** ρ_c (SI unit: $\mathrm{kg/m^3}$) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case the default is 1000 $\mathrm{kg/m^3}$.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref}, which are specified in the Model Input section.

The default **Dynamic viscosity, continuous phase** μ_c (SI unit: Pa·s), uses values **From material**. It describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as

thick, such as oil, have a higher viscosity. For **User defined** enter another value or expression. In this case, the default is 0.001 Pa·s.

DISPERSED PHASE PROPERTIES

The number of **Dispersed Phase Properties** sections depends on the number of phases defined in the coupled Phase Transport interface: the number of sections is equal to the number of dispersed phases, which is in turn equal to the number of phases defined in the coupled Phase Transport interface minus one.

The options in these sections are influenced by the selections made in the **Physical Model** section.

Select the fluid materials to use for the material properties. The default material used for the **Phase** is the **Domain material**.

The default **Density, dispersed phase** ρ_i (SI unit: $\mathrm{kg/m^3}$) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case, the default is 1000 $\mathrm{kg/m^3}$.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref}, which are specified in the Model Input section.

If **Liquid droplets/bubbles** is selected from the **Dispersed phase** list in the **Physical Model** section, then **Dynamic viscosity, dispersed phase** μ_i (SI unit: Pa·s) is also available. The default uses values **From material** or select **User defined** to enter another value or expression. In this case, the default is 0.001 Pa·s.

If one of the predefined slip models (**Hadamard-Rybczynski**, **Schiller-Naumann**, or **Haider-Levenspiel**) is selected from the **Slip model** list in the **Physical Model** section, then **Diameter of particles/droplets** d_i (SI unit: m) is also available. The default is 10^{-3} m (1 mm). If **Haider-Levenspiel** is selected for the **Slip model** under **Physical Model**, enter a value between 0 and 1 for the **Sphericity** (dimensionless). The default is 1.

If a **Schiller-Naumann** or a **Haider-Levenspiel** slip model is selected from the **Slip model** list in the **Physical Model** section, enter an initial value for the **Squared slip velocity** $\mathrm{slipvel}_{0,i}$ (SI unit: $\mathrm{m^2/s^2}$). The default is 0 $\mathrm{m^2/s^2}$.

When a **User defined Slip model** is selected in the **Physical Model** section, specify an arbitrary expression for the slip velocity $\mathbf{u}_{\mathrm{slip},i}$ (SI unit: m/s). For example, give a constant velocity based on experimental data.

- See Theory for the Phase Transport Mixture Model Interfaces

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Phase transport** or **Fluid flow** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

The Nonisothermal Mixture Model Interfaces

The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the **Fluid Flow** > **Multiphase Flow** > **Nonisothermal Mixture Model** branch of the **Model Wizard** or **Add Physics** windows, one of the **Single-Phase Flow** interfaces (laminar or turbulent flow), the **Phase Transport** interface, and the **Heat Transfer in Fluids interfaces** are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling features **Nonisothermal Flow**, **Mixture Model**, and **Nonisothermal Mixture Model**.

The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

- The **Laminar Flow** interface () combines a Laminar Flow interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, Algebraic yPlus** interface () combines a Turbulent Flow, Algebraic yPlus with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, L-VEL** interface () combines a Turbulent Flow, L-VEL interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, k-ε** interface () combines a Turbulent Flow, k-ε interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, Realizable k-ε** interface () combines a Turbulent Flow, Realizable k-ε interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, k-ω** interface () combines a Turbulent Flow, k-ω interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, SST** interface () combines a Turbulent Flow, SST interface with a Phase Transport interface and a Heat Transfer in Fluids interface.

- The **Turbulent Flow, Low Re k-ε** interface ( ) combines a Turbulent Flow, Low Re k-ε interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, Spalart–Allmaras** interface ( ) combines a Turbulent Flow, Spalart–Allmaras interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow, v2-f** interface ( ) combines a Turbulent Flow, v2-f interface with a Phase Transport interface and a Heat Transfer in Fluids interface.

Settings for Physics Interfaces and Coupling Features

When physics interfaces are added using the predefined couplings, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings may not be automatically included.

For example, if single Heat Transfer in Fluids, Phase Transport, and Laminar Flow interfaces are added, COMSOL Multiphysics adds an empty **Multiphysics** node. When you right-click this node, you can add the **Nonisothermal Flow**, **Mixture Model**, or **Nonisothermal Mixture Model** coupling features, but the modified settings are not included. To get all the modified settings presented below automatically, you may

instead right-click the component node, select **Add Multiphysics**, and add **Nonisothermal Mixture Model** from the **Add Multiphysics** window.

TABLE 6-8: MODIFIED SETTINGS FOR THE NONISOTHERMAL FLOW INTERFACES.

PHYSICS OR COUPLING INTERFACE	MODIFIED SETTINGS (IF ANY)
Fluid Flow	Discretization order from temperature Lagrange shape function is 1. The **Compressibility** option of the fluid flow interface is set to **Compressible flow (Ma<0.3)**. The **Temperature**, T (**Model Input** section) is automatically set to the variables from the **Nonisothermal Flow** multiphysics coupling feature.
Phase Transport	The **Absolute pressure**, p_A (**Model Input** section) and the **Velocity field**, $\mathbf{u}$ (**Velocity field** section) are automatically set to the variables from the **Mixture Model** multiphysics coupling feature. **Temperature**, T (**Model Input** section) is automatically set to the variables from the **Nonisothermal Mixture Model** multiphysics coupling feature.
Heat Transfer in Fluids	Discretization order from temperature Lagrange shape function is 1. The **Absolute pressure**, p_A (**Model Input** section) and the **Velocity field**, $\mathbf{u}$ (**Heat Convection** section) are automatically set to the variables from the **Nonisothermal Flow** multiphysics coupling feature.
Nonisothermal Flow	The fluid-flow and heat-transfer interfaces are preselected. The **Specify density** and **Specify reference temperature** settings are set to **From fluid flow interface**.
Mixture Model	The **Phase Transport** and **Fluid Flow** interfaces are preselected.
Nonisothermal Mixture Model	The **Phase Transport** and **Heat transfer** interfaces are preselected.

Coupling Features

Three coupling features are added: The Nonisothermal Flow, the Mixture Model, and the Nonisothermal Mixture Model multiphysics couplings.

Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

PHASE TRANSPORT

The available physics features for The Phase Transport Interface are listed in the section Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, ALGEBRAIC YPLUS

The available physics features for The Turbulent Flow, Algebraic yPlus Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, L-VEL

The available physics features for The Turbulent Flow, L-VEL Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ε

The available physics features for The Turbulent Flow, k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, REALIZABLE k-ε

The available physics features for The Turbulent Flow, Realizable k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ω

The available physics features for The Turbulent Flow, k-ω Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE k-ε

The available physics features for The Turbulent Flow, Low Re k-ε Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SPALART–ALLMARAS

The available physics features for The Turbulent Flow, Spalart–Allmaras Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, V2-F

The available physics features for The Turbulent Flow, v2-f Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

HEAT TRANSFER IN FLUIDS

The available physics features for The Heat Transfer in Fluids Interface are listed in the section The Heat Transfer in Solids and Fluids Interface. Also see Fluid for details about that feature.

Nonisothermal Mixture Model

Use the **Mixture Model** ( ) multiphysics coupling to simulate heat transfers in fluids containing one or more dispersed phases.

The Phase Transport and the Heat Transfer in Fluids interfaces, which are coupled by the **Nonsiothermal Mixture Model** multiphysics coupling, solve together for conservation of mass of the dispersed phases and heat transfer in the mixture.

The Nonisothermal Mixture Model multiphysics coupling provides the mixture thermal conductivity, heat capacity at constant pressure, and ratio of specific heats to the heat transfer interface.

In the Phase Transport interface, it sets the **Temperature** in the **Model Input** section. When the Nonisothermal Mixture Model multiphysics coupling is used together with a **Mixture Model** multiphysics coupling that couples the Phase Transport interface with a single-phase flow interface (laminar or turbulent), it also sets the **Temperature** in the **Model Input** section of the Mixture Model coupling.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `nitmm1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the mixture model, or select **All domains** as needed.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Phase transport** and **Heat Transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Phase Transport** is deleted, then the **Phase transport** list defaults to **None** as there is nothing to couple to.

MODEL INPUTS

The thermal conductivity, heat capacity at constant pressure, and ratio of specific heats of each phase can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

This input appears when a material requires the temperature as a model input. By default, the **Temperature** model input is set from the **Heat Transfer** interface.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. The **Absolute Pressure** model input is per default computed from the Heat Transfer interface. If the Heat Transfer interface is coupled to a single-phase flow (laminar or turbulent) interface using the **Nonisothermal Flow** multiphysics coupling, the absolute pressure will be taken from the single-phase flow interface.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

CONTINUOUS PHASE PROPERTIES

Select the fluid materials to use for the material properties of the continuous phase. The default material used for the **Continuous phase** is the **Domain material**.

Heat conduction

The default **Thermal conductivity** k_c (SI unit: W/(m·K)) uses values **From material** (as selected in the **Materials** section for the **Continuous Phase Properties**). For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the thermal conductivity, and enter values or expressions f or the thermal conductivity or its components. For **Isotropic** enter a scalar which will be used to define a diagonal tensor.

In this case the default is 0 W/(m·K). For the other options, enter values or expressions into the editable fields of the tensor.

Fluid Material

Both the heat capacity at constant pressure $C_{p,c}$ and ratio of specific heats γ_c of the continuous phase can be defined.

The default **Heat capacity at constant pressure** $C_{p,c}$ (SI unit: J/(kg·K)), uses values **From material**. It describes the amount of heat energy required to produce a unit temperature change in a unit mass. For **User defined** enter another value or expression. In this case, the default is 0 J/(kg·K).

The default **Ratio of specific heat** γ_c (SI unit: 1), uses values **From material**. It is the ratio of the heat capacity at constant pressure of the phase, $C_{p,c}$, to the heat capacity at constant volume, $C_{v,c}$. For **User defined** enter another value or expression. In this case, the default is 1. For common diatomic gases such as air, $\gamma = 1.4$ is the standard value. Most liquids have $\gamma = 1.1$ while water has $\gamma = 1.0$. γ is used in the streamline stabilization and in the variables for heat fluxes and total energy fluxes.

DISPERSED PHASE PROPERTIES

The number of **Dispersed Phase Properties** sections depends on the number of phases defined in the coupled Phase Transport interface: the number of sections is equal to the number of dispersed phases, which is in turn equal to the number of phases defined in the coupled Phase Transport interface minus one.

Select the fluid materials to use for the material properties of the phase. The default material used for the **Phase** is the **Domain material**.

Heat conduction

The default **Thermal conductivity** k_d (SI unit: W/(m·K)) uses values **From material** (as selected in the **Materials** section for the **Dispersed Phase Properties**). For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the thermal conductivity, and enter values or expressions for the thermal conductivity or its components. For **Isotropic** enter a scalar which will be used to define a diagonal tensor. In this case the default is 0 W/(m·K). For the other options, enter values or expressions into the editable fields of the tensor.

Fluid Material

Both the heat capacity at constant pressure $C_{p,d}$ and ratio of specific heats γ_d of the phase can be defined.

The default **Heat capacity at constant pressure** $C_{p,d}$ (SI unit: J/(kg·K)), uses values **From material**. It describes the amount of heat energy required to produce a unit temperature change in a unit mass. For **User defined** enter another value or expression. In this case, the default is 0 J/(kg·K).

The default **Ratio of specific heat** γ_d (SI unit: 1), uses values **From material**. It is the ratio of the heat capacity at constant pressure of the phase, $C_{p,d}$, to the heat capacity at constant volume, $C_{v,d}$. For **User defined** enter another value or expression. In this case, the default is 1. For common diatomic gases such as air, $\gamma = 1.4$ is the standard value. Most liquids have $\gamma = 1.1$ while water has $\gamma = 1.0$. γ is used in the streamline stabilization and in the variables for heat fluxes and total energy fluxes.

- See Theory for the Nonisothermal Mixture Model Interfaces
- See Theory for the Phase Transport Mixture Model Interfaces
- See Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Phase transport** or **Fluid flow** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

Theory for the Two-Phase Flow Interfaces

The Two-Phase Flow, Level Set and Phase Field interfaces can be used to model the flow of two different, immiscible fluids, where the exact position of the interface between the two fluids is of interest. The fluid-fluid interface is tracked using an auxiliary function on a fixed mesh. These methods account for differences in the two fluids' densities and viscosities and include the effects of surface tension and gravity.

The Two-Phase Flow, Level Set and Phase Field Interfaces theory is described in this section:

- Level Set and Phase Field Equations
- Conservative and Nonconservative Formulations
- Phase Initialization
- Numerical Stabilization
- References for the Level Set and Phase Field Interfaces

Level Set and Phase Field Equations

By default, the Level Set and Phase Field interfaces use the incompressible formulation of the Navier–Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)] + \mathbf{F}_g + \mathbf{F}_{st} + \mathbf{F}_{ext} + \mathbf{F} \qquad (6\text{-}4)$$

$$\nabla\cdot\mathbf{u} = 0 \qquad (6\text{-}5)$$

Note that Equation 6-4, and Equation 6-5 are solved in the contained interface, **Laminar Flow** or **Turbulent Flow** interface. Note that the form of the continuity equation, appropriate for high density difference mixtures, differs from the definition in Theory for the Single-Phase Flow Interfaces.

USING THE LEVEL SET METHOD

If the level set method is used to track the interface, it adds the following equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{6-6}$$

where γ is the reinitialization parameter (set to 1 by default), and ε is the interface thickness controlling parameter (set proportional to $h_{\max}$ where $h_{\max}$ is the maximum element size in the component). The density is a function of the level set function. Let ρ_1 and ρ_2 be the constant densities of Fluid 1 and Fluid 2, respectively. Here, Fluid 1 corresponds to the domain where $\phi < 0.5$, and Fluid 2 corresponds to the domain where $\phi > 0.5$. When **Density averaging** is set to **Volume average**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$

switching to **Heaviside function**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1) H\left(\frac{\phi - 0{,}5}{l_\rho} \right)$$

where H is a smooth step function and l_ρ is a mixing parameter defining the size of the transition zone. When the **Harmonic volume average** is selected,

$$\rho = \frac{1}{(1-\phi)/\rho_1 + \phi/\rho_2}$$

Similarly, the dynamic viscosity can be defined by setting **Viscosity averaging** to **Volume average**,

$$\mu = \mu_1 + (\mu_2 - \mu_1)\phi$$

Heaviside function,

$$\mu = \mu_1 + (\mu_2 - \mu_1) H\left(\frac{\phi - 0{,}5}{l_\mu} \right)$$

Harmonic volume average,

$$\mu = \frac{1}{(1-\phi)/\mu_1 + \phi/\mu_2}$$

Mass average,

$$\mu = \frac{\rho_1(1-\phi)\mu_1 + \rho_2 \phi \mu_2}{\rho}$$

or **Harmonic mass average**,

$$\mu = \frac{\rho}{\rho_1(1-\phi)/\mu_1 + \rho_2\phi/\mu_2}$$

where μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively. For inelastic non-Newtonian fluids, $\mu_{1,2}$ is replaced by $\mu_{app1,2}$ in the previous expressions. Further details of the theory for the level set method are in Ref. 1.

USING THE PHASE FIELD METHOD

If the phase field method is used to track the interface, it adds the following equations:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \frac{\gamma \lambda}{\varepsilon^2} \nabla \psi \tag{6-7}$$

$$\psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f_{\text{ext}}}{\partial \phi} \tag{6-8}$$

where the quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon}$$

and γ is the mobility parameter which is related to ε through $\gamma = \chi\varepsilon^2$ where χ is the mobility tuning parameter (set to 1 by default). The volume fractions of Fluid 1 and Fluid 2 are computed as

$$V_{f,2} = \min(\max([(1+\phi)/2], 0), 1), \qquad V_{f,1} = 1 - V_{f,2}$$

where the `min` and `max` operators are used so that the volume fractions have a lower limit of 0 and an upper limit of 1. Let ρ_1 and ρ_2 be the constant densities of Fluid 1 and Fluid 2, respectively. When **Density averaging** is set to **Volume average**, the density is defined as,

$$\rho = \rho_1 V_{f,1} + \rho_2 V_{f,2}$$

switching to **Heaviside function**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1)\mathrm{H}\left(\frac{V_{f,2} - 0{,}5}{l_\rho}\right)$$

where H is a smooth step function and l_ρ is a mixing parameter defining the size of the transition zone. When the **Harmonic volume average** is selected,

$$\rho = \frac{1}{V_{f,1}/\rho_1 + V_{f,2}/\rho_2}$$

Similarly, the dynamic viscosity can be defined by setting **Viscosity averaging** to **Volume average**,

$$\mu = V_{f,1}\mu_1 + \mu_2 V_{f,2}$$

Heaviside function,

$$\mu = \mu_1 + (\mu_2 - \mu_1)\mathrm{H}\left(\frac{V_{f,2} - 0{,}5}{l_\mu}\right)$$

Harmonic volume average,

$$\mu = \frac{1}{V_{f,1}/\mu_1 + V_{f,2}/\mu_2}$$

Mass average,

$$\mu = \frac{\rho_1 V_{f,1}\mu_1 + \rho_2 V_{f,2}\mu_2}{\rho}$$

or **Harmonic mass average**,

$$\mu = \frac{\rho}{\rho_1 V_{f,1}/\mu_1 + \rho_2 V_{f,2}/\mu_2}$$

where μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively. For inelastic non-Newtonian fluids, $\mu_{1,2}$ are replaced by $\mu_{app1,2}$ in the previous expressions.

The mean curvature (SI unit: 1/m) can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

where G is the chemical potential defined as:

$$G = \lambda\left(-\nabla^2\phi + \frac{\phi(\phi^2-1)}{\varepsilon^2}\right) + \frac{\partial f}{\partial \phi}$$

Details of the theory for the phase field method are found in Ref. 2.

FORCE TERMS

The four forces on the right-hand side of Equation 6-4 are due to gravity, surface tension, a force due to an external contribution to the free energy (using the phase field method only), and a user-defined volume force.

The Surface Tension Force for the Level Set Method

For the level set method, the surface tension force acting on the interface between the two fluids is:

$$\mathbf{F}_{\text{st}} = \sigma\delta\kappa\mathbf{n} + \delta\nabla_s\sigma$$

where σ is the surface tensions coefficient (SI unit: N/m), $\mathbf{n}$ is the unit normal to the interface, and $\kappa = -\nabla \cdot \mathbf{n}$ is the curvature. δ (SI unit: 1/m) is a Dirac delta function located at the interface. ∇_s is the surface gradient operator

$$\nabla_s = (\mathbf{I} - \mathbf{n}\mathbf{n}^T)\nabla$$

The δ-function is approximated by a smooth function according to

$$\delta = 6|\nabla\phi||\phi(1-\phi)|$$

The Surface Tension Force for the Phase Field Method

The surface tension force for the phase field method is implemented as a body force

$$\mathbf{F}_{\text{st}} = \left(G - \frac{\partial f}{\partial \phi}\right)\nabla\phi$$

where G is the chemical potential (SI unit: J/m^3) defined in The Equations for the Phase Field Method and $\partial f/\partial\phi$ is a user-defined source of free energy. When **Shift surface tension force to the heaviest phase** is selected the surface-tension force is added as,

$$\mathbf{F}_{\text{st}} = \frac{2}{\rho_1+\rho_2}\left(\rho_1 H\left(\frac{V_{\text{f},1}-0.5}{d_{s,Fst}}\right) + \rho_2 H\left(\frac{V_{\text{f},2}-0.5}{d_{s,Fst}}\right)\right)\left(G - \frac{\partial f}{\partial \phi}\right)\nabla\phi$$

where $d_{s,Fst}$ is a smoothing factor. This can be used to avoid unphysical acceleration of a light phase near a phase interface caused by the smearing of the phase interface across a few mesh cells.

If **Include surface tension gradient effects in surface tension force** is selected, extra terms are added to account for the Marangoni effect due to gradients in the surface tension coefficient (see Ref. 6):

$$\mathbf{F}_{\text{st}} = \left(G - \frac{\partial f}{\partial \phi}\right)\nabla\phi + \left(\frac{|\nabla\phi|^2}{2\partial\phi} + \frac{(\phi^2-1)^2}{4\varepsilon^2}\right)\nabla\lambda - (\nabla\lambda\cdot\nabla\phi)\nabla\phi$$

The Gravity Force

The gravity force is $\mathbf{F}_g = \rho\mathbf{g}$ where $\mathbf{g}$ is the gravity vector. Add this as a Gravity feature to the fluid domain.

The User-Defined Volume Force

When using a Phase Field interface, a force arising due to a user-defined source of free energy is computed according to:

$$\mathbf{F}_{\text{ext}} = \left(\frac{\partial f}{\partial \phi}\right)\nabla\phi$$

This force is added when a ϕ-derivative of the external free energy has been defined in the External Free Energy section of the Fluid Properties feature.

Conservative and Nonconservative Formulations

When the velocity field is divergence free, you can use either the conservative or the nonconservative formulation of the level set or phase field equation. The conservative form perfectly conserves the mass of each fluid, but the computational time is generally longer.

When the Level Set or Phase Field in Fluids interface are coupled to a fluid flow interface by means of The Two-Phase Flow, Level Set Coupling Feature or The Two-Phase Flow, Phase Field Coupling Feature, improved conservation of the integral of the level set or phase field variable is obtained using the nonconservative form provided that the discretization order of the level set or phase field variable is equal to or lower than the order of the pressure.

Phase Initialization

If the study type Transient with Phase Initialization is used in the model, the level set or phase field variable is automatically initialized. For this study, two study steps are created: Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the level set function according to the expression

$$\phi_0 = \frac{1}{1 + e^{D_{\text{wi}}/\varepsilon}}$$

in domains initially filled with Fluid 1 and

$$\phi_0 = \frac{1}{1 + e^{-D_{\text{wi}}/\varepsilon}}$$

in domains initially filled with Fluid 2.

Correspondingly, the phase field method uses the expressions

$$\phi_0 = -\tanh\left(\frac{D_{\text{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{\text{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 2. The initial condition for the help variable is $\psi_0 = 0$. These expressions are based on the analytical solution of the steady state solution of Equation 6-6, Equation 6-7, and Equation 6-8 for a straight, nonmoving interface.

If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid 1** and the other **Specify phase: Fluid 2**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. Note that when the value of **Level set variable** or **Phase field variable** is set to **User defined**, arbitrary user defined initial values have to be provided. In this case, the smooth initialization is not used, and a Time Dependent study should be used instead of Time Dependent with Phase Initialization.

- The Two-Phase Flow, Level Set and Phase Field Interfaces
- Studies and Solvers and Time Dependent with Phase Initialization in the *COMSOL Multiphysics Reference Manual*

Numerical Stabilization

Three types of stabilization methods are available for the flow (Navier–Stokes), turbulence, and interface (level set or phase field) equations. Two are consistent stabilization methods — Streamline diffusion and Crosswind diffusion — and one is inconsistent — Isotropic diffusion.

To display this section, click the **Show More Options** button ( ) and select **Stabilization** from the **Show More Options** dialog.

- The Two-Phase Flow, Level Set and Phase Field Interfaces
- Selection Information in the *COMSOL Multiphysics Reference Manual*

References for the Level Set and Phase Field Interfaces

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Theory for the Two-Phase Thin-Film Flow, Phase Field Interfaces

The Two-Phase Thin-Film Flow, Phase Field interfaces can be used to model the flow of two different, immiscible fluids in thin, narrow channels, where the exact position of the interface between the two fluids is of interest. The fluid-fluid interface is tracked using an auxiliary function on a fixed mesh. These methods account for differences in the two fluids' densities and viscosities and include the effects of surface tension.

The Two-Phase Thin-Film Flow, Phase Field Interfaces' theory is described in this section:

- Phase Field Thin-Film Flow Equations
- Conservative and Nonconservative Formulations
- Phase Initialization
- References for the Phase Field Thin-Film Flow Interfaces

Phase Field Thin-Film Flow Equations

The phase field method, used to track the interface, adds the following equations:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla_t \phi = \nabla_t \cdot \frac{\gamma \lambda}{\varepsilon^2} \nabla_t \psi \tag{6-9}$$

$$\psi = -\nabla_t \cdot \varepsilon^2 \nabla_t \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right) \frac{\partial f_{\text{ext}}}{\partial \phi} \tag{6-10}$$

where the quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3} \frac{\lambda}{\varepsilon}$$

and γ is the mobility parameter which is related to ε through $\gamma = \chi \varepsilon^2$ where χ is the mobility tuning parameter (set to 1 by default). The volume fractions of Fluid 1 and Fluid 2 are computed as

$$V_{f,2} = \min(\max([(1+\phi)/2], 0), 1), \qquad V_{f,1} = 1 - V_{f,2}$$

where the `min` and `max` operators are used so that the volume fractions have a lower limit of 0 and an upper limit of 1. Let ρ_1 and ρ_2 be the constant densities of Fluid 1 and Fluid 2, respectively. When **Density averaging** is set to **Volume average**, the density is defined as,

$$\rho = \rho_1 V_{f,1} + \rho_2 V_{f,2}$$

switching to **Heaviside function**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1) H\left(\frac{V_{f,2} - 0{,}5}{l_\rho}\right)$$

where H is a smooth step function and l_ρ is a mixing parameter defining the size of the transition zone. When the **Harmonic volume average** is selected,

$$\rho = \frac{1}{V_{f,1}/\rho_1 + V_{f,2}/\rho_2}$$

Similarly, the dynamic viscosity can be defined by setting **Viscosity averaging** to **Volume average**,

$$\mu = V_{f,1}\mu_1 + \mu_2 V_{f,2}$$

Heaviside function,

$$\mu = \mu_1 + (\mu_2 - \mu_1) H\left(\frac{V_{f,2} - 0{,}5}{l_\mu}\right)$$

Harmonic volume average,

$$\mu = \frac{1}{V_{f,1}/\mu_1 + V_{f,2}/\mu_2}$$

Mass average,

$$\mu = \frac{\rho_1 V_{f,1}\mu_1 + \rho_2 V_{f,2}\mu_2}{\rho}$$

or **Harmonic mass average**,

$$\mu = \frac{\rho}{\rho_1 V_{f,1}/\mu_1 + \rho_2 V_{f,2}/\mu_2}$$

where μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively.

The mean curvature (SI unit: 1/m) can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

where G is the chemical potential defined as:

$$G = \lambda\left(-\nabla_t{}^2\phi + \frac{\phi(\phi^2-1)}{\varepsilon^2}\right) + \frac{\partial f}{\partial \phi}$$

Details of the theory for the phase field method are found in Ref. 2.

FORCE TERMS

The forces applied on the right-hand side of the momentum equation are due to surface tension and a user-defined volume force.

The Surface Tension Force for the Phase Field Method

The surface tension force for the phase field method is implemented as a body force

$$F_{st} = \left(G - \frac{\partial f}{\partial \phi}\right)\nabla_t \phi$$

where G is the chemical potential (SI unit: J/m^3) defined in The Equations for the Phase Field Method and $\partial f/\partial\phi$ is a user-defined source of free energy.

The User-Defined Volume Force

When using a Phase Field in Fluids interface, a force arising due to a user-defined source of free energy is computed according to:

$$\mathbf{F}_{ext} = \left(\frac{\partial f}{\partial \phi}\right)\nabla_t \phi$$

This force is added when a ϕ-derivative of the external free energy has been defined in the External Free Energy section of the Fluid Properties feature.

Conservative and Nonconservative Formulations

When the velocity field is divergence free, you can use either the conservative or the nonconservative formulation of the phase field thin-film flow equation. The conservative form perfectly conserves the mass of each fluid, but the computational time is generally longer.

When the Phase Field Thin-Film Flow interface are coupled to a Thin-Film Flow interface through The Two-Phase Thin-Film Flow, Phase Field Coupling Feature, improved conservation of the integral of the phase field variable is obtained using the nonconservative form provided that the discretization order of the phase field variable is equal to or lower than the order of the film pressure.

Phase Initialization

If the study type Transient with Phase Initialization is used in the model, the phase field variable is automatically initialized. For this study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the level set function according to the following expression:

$$\phi_0 = \frac{1}{1 + e^{D_{\mathrm{wi}}/\varepsilon}}$$

in domains initially filled with Fluid 1 and

$$\phi_0 = \frac{1}{1 + e^{-D_{\mathrm{wi}}/\varepsilon}}$$

in domains initially filled with Fluid 2.

Correspondingly, for the phase field method the following expressions are used:

$$\phi_0 = -\tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 2. The initial condition for the help variable is $\psi_0 = 0$. These expressions are based on the analytical solution of the steady state solution of Equation 6-9, and Equation 6-10 for a straight, nonmoving interface.

If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid 1** and the other **Specify phase: Fluid 2**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. Note that when the value of **Phase field variable** is set to **User defined**, arbitrary user defined initial values have to be provided. In this case, the smooth initialization is not used, and a Time Dependent study should be used instead of Time Dependent with Phase Initialization.

- The Two-Phase Thin-Film Flow, Phase Field Interfaces
- Studies and Solvers and Time Dependent with Phase Initialization in the *COMSOL Multiphysics Reference Manual*

References for the Phase Field Thin-Film Flow Interfaces

See References for the Level Set and Phase Field Interfaces.

Theory for the Three-Phase Flow Interface

The Three-Phase Flow, Phase Field interface can be used to model the flow and interaction of three different, immiscible fluids, when the exact positions of the interfaces separating the fluids are of interest. The fluid-fluid interfaces are tracked using a ternary phase field formulation which account for differences in the fluids' densities and viscosities and include the effects of surface tension.

The Two-Phase Thin-Film Flow, Phase Field Interfaces theory is described in the following sections:

- Governing Equations of the Three-Phase Flow, Phase Field Interface
- Reference for the Three-Phase Flow, Phase Field Interface

Governing Equations of the Three-Phase Flow, Phase Field Interface

LAMINAR FLOW EQUATIONS

The Three-Phase Flow, Phase Field interface is used to study the evolution of three immiscible fluid phases denoted by fluid A, fluid B, and fluid C. The interface solves the Navier–Stokes equations governing conservation of momentum and mass. The momentum equations solved correspond to

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] + \mathbf{F}_{\mathrm{st}} + \mathbf{F} \quad (6\text{-}11)$$

where $\mathbf{F}_{\mathrm{st}}$ is the surface tension force. The physics interface assumes that the density of each phase is constant. The density may however vary between the phases. In order to accurately handle systems where density of the phases are significantly different, as well as systems with phases of similar density, the following fully compressible continuity equation is solved by the interface

$$\frac{\partial \log\rho}{\partial t} + \nabla\cdot\mathbf{u} + \mathbf{u}\cdot\nabla\log\rho = 0 \quad (6\text{-}12)$$

TERNARY PHASE-FIELD EQUATIONS

In order to track the interfaces between three immiscible fluids, a ternary phase field model based on the work of Boyer and co-workers in Ref. 1 is used. The model solves the following Cahn–Hilliard equations

$$\begin{aligned}\frac{\partial \phi_i}{\partial t} + \nabla \cdot (\mathbf{u}\phi_i) &= \nabla \cdot \left(\frac{M_0}{\Sigma_i}\nabla \eta_i\right) \\ \eta_i &= \frac{4\Sigma_{\mathrm{T}}}{\varepsilon}\sum_{j \neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial \phi_i} - \frac{\partial F}{\partial \phi_j}\right)\right) - \frac{3}{4}\varepsilon\Sigma_j\nabla^2\phi_i\end{aligned} \tag{6-13}$$

governing the phase field variable, ϕ_i, and a generalized chemical potential, η_i, of each phase $i = A, B, C$. The phase field variables vary between 0 and 1 and are a measure of the concentration of each phase. The phase field variable for phase A is one in instances containing only this phase, and zero where there is no phase A. Since the fluids are immiscible, variations in the phase field variable occur, and define the interface separating two phases. At each point the phase field variables satisfy the following constraint

$$\sum_{i = A, B, C} \phi_i = 1 \tag{6-14}$$

The density of each phase is assumed to be constant which implies that the phase field variable corresponds to the volume fraction of the phase in question. In order to satisfy Equation 6-14, two sets of the equations shown in Equation 6-13 are solved, namely those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 6-14.

The density and viscosity of the fluid mixture used in Equation 6-4 and 6-5 are defined as:

$$\begin{aligned}\rho &= \rho_A\phi_A + \rho_B\phi_B + \rho_C\phi_C \\ \mu &= \mu_A\phi_A + \mu_B\phi_B + \mu_C\phi_C\end{aligned} \tag{6-15}$$

Free Energy

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$F = \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 + \phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2 \tag{6-16}$$

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase i and j, and the capillary parameters Σ_i are defined for each phase in the manner of:

$$\begin{aligned}\Sigma_A &= \sigma_{AB} + \sigma_{AC} - \sigma_{BC}\\ \Sigma_B &= \sigma_{AB} + \sigma_{BC} - \sigma_{AC}\\ \Sigma_C &= \sigma_{BC} + \sigma_{AC} - \sigma_{AB}\end{aligned} \tag{6-17}$$

Λ in the free energy is a function or parameter specifying the additional free bulk energy of the system. By default Λ is zero. In this case it can be seen that the free energy in Equation 6-16 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

Ternary Phase Field Parameters

In Equation 6-13, ε (SI unit: $1/\mathrm{m}$) is a parameter controlling the interface thickness, M_0 (SI unit: m^3/s) is a molecular mobility parameter, and the parameter Σ_T is defined as

$$\frac{3}{\Sigma_\mathrm{T}} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \tag{6-18}$$

When using the interface it is recommended that the parameter ε is given a value in the same order as the elements in the regions passed by the fluid-fluid interfaces. The mobility determines the time scale of the Cahn–Hilliard diffusion and must be large enough to retain a constant interfacial thickness, but small enough to avoid damping the convective transport. In order to ensure that the mobility is in the correct range, it is recommended to apply a mobility parameter such that the following holds approximately

$$M_0 = L_c U_c \varepsilon \cdot 10^{-2} \tag{6-19}$$

where L_c and U_c are the characteristic length and velocity scales of the system at hand.

SURFACE TENSION

The surface tension force applied in the momentum equations (Equation 6-4) as a body force computed from the generalized chemical potentials:

$$\mathbf{F}_{\mathrm{st}} = \sum_{i = \mathrm{A}, B, C} \eta_i \nabla \phi_i \tag{6-20}$$

Reference for the Three-Phase Flow, Phase Field Interface

1. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar, and M. Quintard, "Cahn-Hilliard/ Navier–Stokes model for the simulation of three-phase flows," *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

Theory for the Two-Phase Flow, Moving Mesh Interface

The Laminar Two-Phase Flow, Moving Mesh Interface can be used to model the flow of two different, immiscible fluids, when the exact position of the interface is of interest. The interface position is tracked by a moving mesh, with boundary conditions that account for surface tension and wetting, as well as mass transport across the interface.

In this section:

- Domain Level Fluid Flow
- About the Moving Mesh
- About the Fluid Interface Boundary Conditions
- Contact Angle Boundary Conditions
- References for the Two-Phase Flow, Moving Mesh Interface

Domain Level Fluid Flow

Two Phase Flow Moving Mesh interface is a predefined physics interface coupling between a Single-Phase Flow interface and the Moving Mesh interface. Within the domains corresponding to individual phases the fluid flow is solved using the Navier–Stokes equations as in the Laminar Flow interface. The general form for the isothermal Navier–Stokes equations is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F}$$

where:

- ρ is the density (SI unit: kg/m^3)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- p is pressure (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: N/m^3)

- τ is the viscous stress tensor (SI unit: Pa).

For a Newtonian fluid the viscous stress tensor, τ, is given by:

$$\tau = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \tag{6-21}$$

The dynamic viscosity μ (SI unit: Pa·s) is allowed to depend on the thermodynamic state but not on the velocity field.

Theory for the Single-Phase Flow Interfaces

About the Moving Mesh

The mesh within the fluid flow domain is deformed to account for the movement of the interface between the two fluids. The software perturbs the mesh nodes so they conform with the moving interface and with other moving or stationary boundaries in the model. The boundary displacement is propagated throughout the domain to obtain a smooth mesh deformation everywhere. This is done by solving equations for the mesh displacements (a Laplace, Winslow, or hyperelastic smoothing equation). Taking two dimensions as an example, a location in the deformed mesh with coordinates (x, y) can be related to its coordinates in the original undeformed mesh (X, Y) by a function of the form:

$$x = x(X, Y, t), \qquad y = y(X, Y, t)$$

The original, undeformed, mesh is referred to as the *material frame* (or reference frame) whilst the deformed mesh is called the *spatial frame*. COMSOL Multiphysics also defines *geometry* and *mesh frames*, which are coincident with the material frame for this physics interface.

The fluid flow equations (along with other coupled equations such as electric fields or chemical species transport) are solved in the spatial frame in which the mesh is perturbed. The movement of the phase boundary is therefore accounted for in these interfaces.

Deformed Geometry and Moving Mesh in the *COMSOL Multiphysics Reference Manual*

The interfaces between phases are tracked with specific boundary conditions for the mesh displacement and the fluid flow. Two options are available — Free Surface and Fluid-Fluid Interface. The Free Surface boundary condition is appropriate when the viscosity of the external fluid is negligible compared to that of the internal fluid. In this case the pressure of the external fluid is the only parameter required to model the fluid and the flow is not solved for in the external fluid. For a fluid-fluid interface the flow is solved for both phases.

FLUID-FLUID INTERFACE

The boundary conditions applied at an interface between two immiscible fluids, fluid 1 and fluid 2 (see Figure 6-2), are given by (Ref. 1):

$$\mathbf{u}_1 = \mathbf{u}_2 + \left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right) M_f \mathbf{n}_i \tag{6-22}$$

$$\mathbf{n}_i \cdot \tau_2 = \mathbf{n}_i \cdot \tau_1 + \mathbf{f}_{st} \tag{6-23}$$

$$\mathbf{u}_{\text{mesh}} = \left(\mathbf{u}_1 \cdot \mathbf{n}_i - \frac{M_f}{\rho_1}\right) \mathbf{n}_i \tag{6-24}$$

where $\mathbf{u}_1$ and $\mathbf{u}_2$ are the velocities of the fluids 1 and 2 respectively, $\mathbf{u}_{\text{mesh}}$ is the velocity of the mesh at the interface between the two fluids, $\mathbf{n}_i$ is the normal of the interface (outward from the domain of fluid 1), τ_1 and τ_2 are the total stress tensors in domains 1 and 2 respectively, $\mathbf{f}_{st}$ is the force per unit area due to the surface tension and M_f is the mass flux across the interface (SI unit: kg/(m^{2}s)).

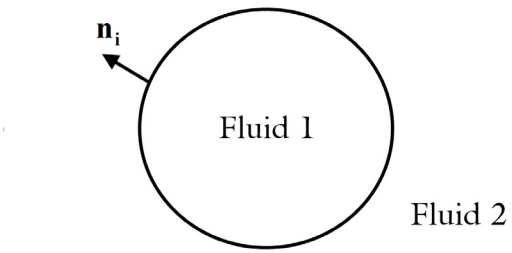

Figure 6-2: Definition of fluid 1 and fluid 2 and the interface normal.

The tangential components of Equation 6-22 enforce a no-slip condition between the fluids at the boundary. In the absence of mass transfer across the boundary, Equation 6-22 and Equation 6-24 ensure that the fluid velocity normal to the boundary is equal to the velocity of the interface. When mass transfer occurs these equations result from conservation of mass and are easily derived in the frame where the boundary is stationary.

The components of the total stress tensor, τ_{uv}, represent the u^{th} component of the force per unit area perpendicular to the v direction. $\mathbf{n}\cdot\tau = \mathbf{n}_v\tau_{uv}$ (using the summation convention) is therefore interpreted as the force per unit area acting on the boundary - in general this is not normal to the boundary. Equation 6-23 therefore expresses the force balance on the interface between the two fluids.

Two boundary conditions (Equation 6-22 and Equation 6-23) are necessary to couple the two domains as there are two separate sets of Navier–Stokes equations, one set for each of the domains.

The force due to the surface tension is given by the following expression:

$$\mathbf{f}_{st} = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i - \nabla_s\sigma \tag{6-25}$$

where ∇_s is the surface gradient operator ($\nabla_s = (\mathbf{I} - \mathbf{n}_i\,\mathbf{n}_i^T)\nabla$, where $\mathbf{I}$ is the identity matrix) and σ is the surface tension at the interface.

In the two dimensional case it is straightforward to see the physical origin of Equation 6-25. Consider an element of the surface of unit depth into the page as shown in Figure 6-3. The normal force per unit area $\mathbf{F}_n$ on the element in the limit $\delta s \to 0$ is:

$$\mathbf{F}_n \delta s = (\sigma + \delta\sigma)\sin(\delta\theta) \to \sigma\delta\theta$$

Because $R\delta\theta \to \delta s$ in the limit,

$$\mathbf{F}_n = \frac{\sigma}{R}$$

The quantity $\nabla_s\cdot\mathbf{n}_i$ in the first term on the right-hand side of Equation 6-25 is related to the mean curvature, κ, of the surface by the equation $\kappa = -\nabla_s\cdot\mathbf{n}_i$. In two dimensions the mean curvature $\kappa = -1/R$ so $\nabla_s\cdot\mathbf{n}_i = 1/R$. The first term in Equation 6-25 is therefore the normal force per unit area acting on the boundary due to the surface tension.

The tangential force per unit area, $\mathbf{F}_t$, acting on the interface in Figure 6-3 can be obtained from the force balance along the direction of δs in the limit $\delta s \to 0$:

$$\mathbf{F}_t \delta s = (\sigma + \delta\sigma)\cos(\delta\theta) - \sigma \to (\sigma + \delta\sigma) - \sigma$$

$$\mathbf{F}_t \to \frac{(\sigma + \delta\sigma) - \sigma}{\delta s}$$

This is equivalent to the second term on the right of Equation 6-25.

To obtain additional insight into the boundary condition, it is helpful to rewrite Equation 6-23 as

$$\mathbf{n}_i \cdot ((p_1 - p_2)I - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T) + \mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T)) = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i - \nabla_s\sigma$$

assuming Newtonian fluids with viscosities μ_1 and μ_2 for fluids 1 and 2, respectively, and that p_1 and p_2 are the pressures in the respective fluids adjacent to the boundary. This equation expresses the equality of two vector quantities. It is instructive to consider the components perpendicular and tangential to the boundary. In the direction of the boundary normal

$$p_1 - p_2 + \mathbf{n}_i \cdot (\mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T) - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T)) \cdot \mathbf{n}_i = \sigma(\nabla_s \cdot \mathbf{n}_i) \quad (6\text{-}26)$$

whereas in the tangential direction, $\mathbf{t}_i$,

$$\mathbf{n}_i \cdot (\mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T) - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T)) \cdot \mathbf{t}_i = |\nabla_s\sigma| \quad (6\text{-}27)$$

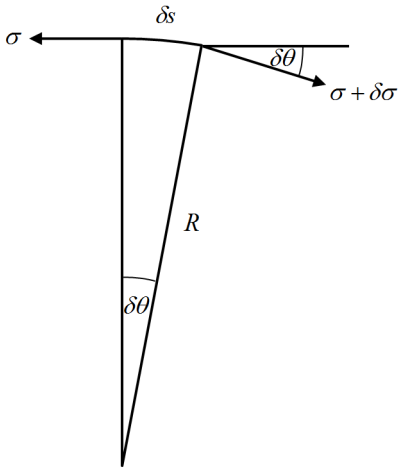

Figure 6-3: Diagrammatic representation of the forces acting on an element of a two-dimensional curved surface.

For the case of a static interface, Equation 6-26 expresses the pressure difference across the interface that results from its curvature. For a moving interface, the surface tension balances the difference in the total normal stress on either side of the interface.

Equation 6-27 involves only velocity gradients and the gradient of the surface tension. The implication of this is that surface tension gradients always drive motion; this is known as the *Marangoni effect*.

FREE SURFACE

It is often the case that the viscosity of fluid 1 is significantly greater than that of fluid 2 (for example for a liquid-vapor interface). In this case, the viscosity terms in the total stress from fluid 2 can be neglected and Equation 6-23 becomes:

$$\mathbf{n}_i \cdot \tau_1 = -p_{\text{ext}}\mathbf{n}_i + \mathbf{f}_{st} \tag{6-28}$$

The outer fluid (fluid 2) now enters the equation system only through the pressure term and the system can be represented by a domain consisting solely of the fluid 1 domain with an expression (or constant value) for the external pressure, p_{ext}, in the fluid 2 domain. Since the velocity in fluid 2 does not affect fluid 1, fluid 2 does not need to be explicitly modeled and Equation 6-22 can be dropped.

Contact Angle Boundary Conditions

At a three-phase boundary, it is necessary to add force terms on the boundary to ensure that the fluid maintains a consistent contact angle. Additionally the Wall boundary condition with the Navier Slip option must be used on the walls. The forces acting on the contact point are applied to the model by the Contact Angle node.

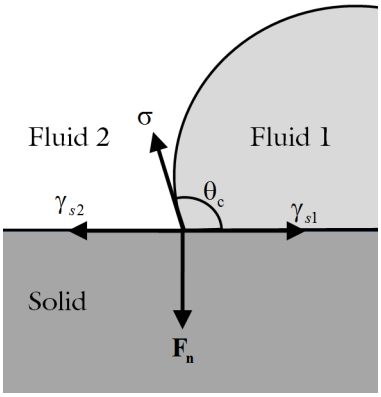

Figure 6-4: Forces per unit length acting on a fluid-fluid interface at a three phase boundary with a solid wall. The surface tension force per unit length, σ, is balanced by a reaction force per unit length at the surface, $\mathbf{F}_n$, and by the forces generated by the surface energies of the two phases at the interface: γ_{s1} and γ_{s2}.

In equilibrium, the surface tension forces and the normal restoring force from the surface are in balance at a constant contact angle (θ_c), as shown in Figure 6-4. This equilibrium is expressed by Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_c) + \gamma_{s1} = \gamma_{s2} \tag{6-29}$$

where σ is the surface tension force between the two fluids, γ_{s1} is the surface energy density on the fluid 1 — solid interface and γ_{s2} is the surface energy density on the fluid 2 — solid interface.

There is still debate in the literature as to precisely what occurs in nonequilibrium situations (for example, drop impact) when the physical contact angle deviates from the contact angle specified by a simple application of Young's equation. A simple approach is to assume that the unbalanced part of the in plane Young Force acts on the fluid to move the contact angle toward its equilibrium value (Ref. 2). COMSOL

Multiphysics employs this approach as it is physically motivated and is consistent with the allowed form of the boundary condition from thermodynamics (Ref. 3 and Ref. 4).

The normal force balance at the solid surface is handled by the wall boundary condition, which automatically prevents fluid flow across the solid boundary by the application of a constraint force. The contact angle feature applies a force on the fluid at the interface, $\mathbf{f}_{wf}$, with magnitude:

$$\mathbf{f}_{wf} = \sigma(\cos(\theta_c) - \cos(\theta))\mathbf{m}_s$$

where θ is the actual contact angle and $\mathbf{m}_s$ is the binormal to the solid surface, as defined in Figure 6-5.

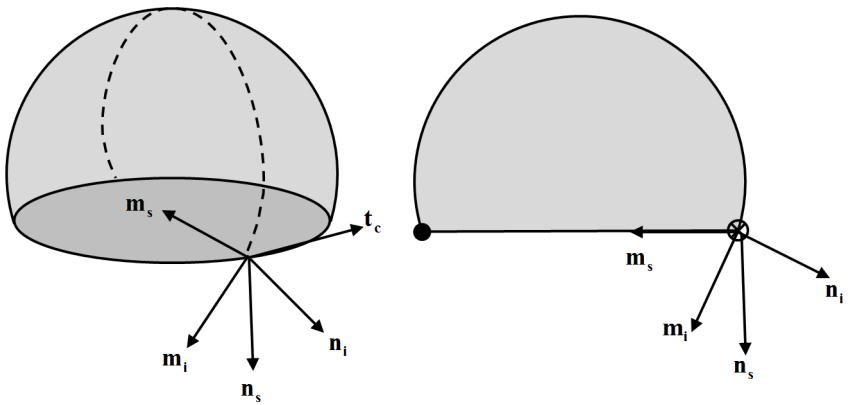

Figure 6-5: Diagram showing normal and tangential vectors defined on the interface between two fluids and a solid surface in 3D (left) and 2D (right). The following vectors are defined: $\mathbf{n}_i$, the fluid-fluid interface unit normal; $\mathbf{n}_s$, the solid surface unit normal; $\mathbf{t}_c$, the tangent to the three-phase contact line; and $\mathbf{m}_i$ and $\mathbf{m}_s$, the two unit binormals, which are defined as $\mathbf{m}_i = \mathbf{t}_c \times \mathbf{n}_i$ and $\mathbf{m}_s = \mathbf{t}_c \times \mathbf{n}_s$, respectively.

References for the Two-Phase Flow, Moving Mesh Interface

1. R. Scardovelli and S. Zaleski, "Direct Numerical Simulation of Free Surface and Interfacial Flow," *Annu. Rev. Fluid Mech.*, vol. 31, pp. 567–603, 1999.

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6. R. C. Weast, ed.,“CRC Handbook of Chemistry and Physics”, ed. 69, MIT Press, 1988.

7. A. G. Gaonkar, “Interfacial Tensions of Vegetable Oil/Water Systems: Effect of Oil Purification”, *J. Am. Oil Chem. Soc*., vol. 66, no. 8, pp. 1090-1092, 1989.

Theory for the Bubbly Flow Interfaces

The Bubbly Flow interfaces are suitable for macroscopic modeling of mixtures of liquids and gas bubbles. These physics interfaces solve for the averaged volume fraction occupied by each of the two phases, rather than tracking each bubble in detail. Each phase has its own velocity field.

In this section:

- The Bubbly Flow Equations
- Turbulence Modeling in Bubbly Flow Applications
- References for the Bubbly Flow Interfaces

The Bubbly Flow Equations

The two-fluid Euler–Euler Model is a general, macroscopic model for two-phase fluid flow. It treats the two phases as interpenetrating media, tracking the averaged concentration of the phases. One velocity field is associated with each phase. A momentum balance equation and a continuity equation describe the dynamics of each of the phases. The *bubbly flow* model is a simplification of the two-fluid model, relying on the following assumptions:

- The gas density is negligible compared to the liquid density.
- The motion of the gas bubbles relative to the liquid is determined by a balance between viscous drag and pressure forces.
- The two phases share the same pressure field.

Based on these assumptions, the momentum and continuity equations for the two phases can be combined and a gas phase transport equation is kept in order to track the volume fraction of the bubbles. The momentum equation is

$$\begin{aligned}\phi_l\rho_l\frac{\partial \mathbf{u}_l}{\partial t} + \phi_l\rho_l\mathbf{u}_l\cdot\nabla\mathbf{u}_l &= \\ = -\nabla p + \nabla\cdot\left[\phi_l(\mu_l+\mu_T)\left(\nabla\mathbf{u}_l+\nabla\mathbf{u}_l^{\,T}-\frac{2}{3}(\nabla\cdot\mathbf{u}_l)\mathbf{I}\right)\right] + \phi_l\rho_l\mathbf{g}+\mathbf{F}\end{aligned} \quad (6\text{-}30)$$

In Equation 6-30, the variables are as follows:

- $\mathbf{u}_l$ is the velocity vector (SI unit: m/s)
- p is the pressure (SI unit: Pa)
- $\phi$is the phase volume fraction (SI unit: m^3/m^3)
- ρ is the density (SI unit: kg/m^3)
- $\mathbf{g}$ is the gravity vector (SI unit: m/s^2)
- $\mathbf{F}$ is any additional volume force (SI unit: N/m^3)
- μ_l is the dynamic viscosity of the liquid (SI unit: Pa·s), and
- μ_T is the turbulent viscosity (SI unit: Pa·s)

The subscripts "l" and "g" denote quantities related to the liquid phase and the gas phase, respectively.

The continuity equation is

$$\frac{\partial}{\partial t}(\rho_l\phi_l + \rho_g\phi_g) + \nabla \cdot (\rho_l\phi_l\mathbf{u}_l + \rho_g\phi_g\mathbf{u}_g) = 0 \tag{6-31}$$

and the gas phase transport equation is

$$\frac{\partial \rho_g\phi_g}{\partial t} + \nabla \cdot (\phi_g\rho_g\mathbf{u}_g) = -m_{gl} \tag{6-32}$$

where m_{gl} is the mass transfer rate from the gas to the liquid (SI unit: $kg/(m^3 \cdot s)$).

For low gas volume fractions ($\phi_g \sim 0.01$), you can replace the momentum equations, Equation 6-30, and the continuity equation, Equation 6-31, by

$$\rho_l\frac{\partial \mathbf{u}_l}{\partial t} + \rho_l\mathbf{u}_l \cdot \nabla\mathbf{u}_l = = -\nabla p + \nabla \cdot [(\mu_l + \mu_T)(\nabla\mathbf{u}_l + \nabla\mathbf{u}_l^T)] + \phi_l\rho_l\mathbf{g} + \mathbf{F} \tag{6-33}$$

$$\rho_l\nabla \cdot \mathbf{u}_l = 0 \tag{6-34}$$

By default, the Laminar Bubbly Flow interface uses Equation 6-33 and 6-34. To switch to Equation 6-30 and 6-31, click to clear the **Low gas concentration** checkbox under the **Physical Model** section.

The physics interface solves for $\mathbf{u}_l$, p, and

$$\tilde{\rho}_g = \rho_g \phi_g$$

the effective gas density. The gas velocity $\mathbf{u}_g$ is the sum of the following velocities:

$$\mathbf{u}_g = \mathbf{u}_l + \mathbf{u}_{slip} + \mathbf{u}_{drift} \tag{6-35}$$

where $\mathbf{u}_{slip}$ is the relative velocity between the phases and $\mathbf{u}_{drift}$ is a drift velocity (see Turbulence Modeling in Bubbly Flow Applications). The physics interface calculates the gas density from the ideal gas law:

$$\rho_g = \frac{(p + p_{ref})M}{RT}$$

where M is the molecular weight of the gas (SI unit: kg/mol), R is the ideal gas constant (8.314472 J/(mol·K)), p_{ref} a reference pressure (SI unit: Pa), and T is temperature (SI unit: K). p_{ref} is a scalar variable, which by default is 1 atm (1 atmosphere or 101,325 Pa). The liquid volume fraction is calculated from

$$\phi_l = 1 - \phi_g$$

When there is a drift velocity, it has the form

$$\mathbf{u}_{drift} = -D_{gc}\frac{\nabla \phi_g}{\phi_g} \tag{6-36}$$

where

$$D_{gc} = \frac{\mu_T}{\rho_l \sigma_T}$$

Here, μ_T is the turbulent viscosity, and σ_T is the turbulent Schmidt number.

Inserting Equation 6-36 and Equation 6-35 into Equation 6-32 gives

$$\frac{\partial \rho_g \phi_g}{\partial t} + \nabla \cdot (\phi_g \rho_g (\mathbf{u}_l + \mathbf{u}_{slip})) = \nabla \cdot (D_{gc}\ \rho_g \nabla \phi_g) - m_{gl}$$

That is, the drift velocity introduces a diffusive term in the gas transport equation. This is how the equation for the transport of the volume fraction of gas is actually implemented in the physics interface.

MASS TRANSFER AND INTERFACIAL AREA

It is possible to account for mass transfer between the two phases by specifying an expression for the mass transfer rate from the gas to the liquid m_{gl} (SI unit: kg/(m^3·s)).

The mass transfer rate typically depends on the interfacial area between the two phases. An example is when gas dissolves into a liquid. In order to determine the interfacial area, it is necessary to solve for the bubble number density (that is, the number of bubbles per volume) in addition to the phase volume fraction. The Bubbly Flow interface assumes that the gas bubbles can expand or shrink but not completely vanish, merge, or split. The conservation of the number density n (SI unit: $1/\text{m}^3$) then gives

$$\frac{\partial n}{\partial t} + \nabla \cdot (n(\mathbf{u}_l + \mathbf{u}_{slip})) = \nabla \cdot (D_{gc} \nabla n)$$

The number density and the volume fraction of gas give the interfacial area per unit volume (SI unit: m^2/m^3):

$$a = (4n\pi)^{1/3}(3\phi_g)^{2/3}$$

SLIP MODEL

The simplest possible approximation for the slip velocity $\mathbf{u}_{slip}$ is to assume that the bubbles always follow the liquid phase; that is, $\mathbf{u}_{slip} = \mathbf{0}$. This is known as homogeneous flow.

A better model can be obtained from the momentum equation for the gas phase. Comparing size of different terms, it can be argued that the equation can be reduced to a balance between the viscous drag force, $\mathbf{f}_D$ and the pressure gradient (Ref. 3), a so called pressure-drag balance:

$$\phi_l \nabla p = \mathbf{f}_D \tag{6-37}$$

Here $\mathbf{f}_D$ can be written as

$$\mathbf{f}_D = -C_d \frac{3}{4} \frac{\rho_l}{d_b} |\mathbf{u}_{slip}| \mathbf{u}_{slip} \tag{6-38}$$

where in turn d_b (SI unit: m) is the bubble diameter, and C_d (dimensionless) is the viscous drag coefficient. Given C_d and d_b, Equation 6-37 can be used to calculate the slip velocity. In practice, Equation 6-37 is multiplied by ϕ_l to reduce the slip velocity for large values of ϕ_g.

Schwarz and Turner (Ref. 4) proposed a linearized version of Equation 6-38 appropriate for air bubbles of 1–10 mm mean diameter in water:

$$\mathbf{f}_D = -C_{\mathrm{W}}\mathbf{u}_{\mathrm{slip}} \quad C_{\mathrm{W}} = 5 \cdot 10^4 \ \frac{\mathrm{kg}}{\mathrm{m}^3 \cdot \mathrm{s}} \tag{6-39}$$

The Hadamard–Rybczynski model is appropriate for small spherical bubbles with diameter less than 2 mm, and bubble Reynolds number less than one. The model uses the following expression for the drag coefficient (Ref. 5):

$$C_{\mathrm{d}} = \frac{16}{\mathrm{Re}_{\mathrm{b}}}, \qquad \mathrm{Re}_{\mathrm{b}} = \frac{d_{\mathrm{b}}\rho_{\mathrm{l}}|\mathbf{u}_{\mathrm{slip}}|}{\mu_{\mathrm{l}}}$$

For bubbles with diameter larger than 2 mm, the model suggested by Sokolichin, Eigenberger, and Lapin (Ref. 1) is a more appropriate choice:

$$C_{\mathrm{d}} = \frac{0{,}622}{\frac{1}{\mathrm{Eö}} + 0{,}235}$$

where Eö is the Eötvös number

$$\mathrm{Eö} = \frac{g\rho_{\mathrm{l}}d_{\mathrm{b}}^2}{\sigma}$$

Here, g is the magnitude of the gravity vector and σ the surface tension coefficient.

Turbulence Modeling in Bubbly Flow Applications

For most *bubbly flow* applications the flow field is turbulent. In that case, use a turbulence model and solve for the averaged velocity field. The Bubbly Flow, Turbulent Flow interfaces include the turbulence models described in Theory for the Turbulent Flow Interfaces, but the material properties of the liquid phase are used. In addition to the options of the single-phase flow model, in The Bubbly Flow, k-ε Interface, The Bubbly Flow, Realizable k-ε Interface, The Bubbly Flow, k-ω Interface, The Bubbly Flow, SST Interface, The Bubbly Flow, Low Re k-ε Interface and The Bubbly Flow, v2-f Interface it is also possible to account for bubble-induced turbulence — that is, extra production of turbulence due to relative motion between the gas bubbles and the liquid. The transport equation for the turbulent kinetic energy, k, includes a source term S_{k} which accounts for bubble-induced turbulence and is given by

$$S_k = -C_k \phi_g \nabla p \cdot \mathbf{u}_{slip}$$

The transport equation for the turbulent energy's dissipation rate, ε, includes the following source term:

$$C_\varepsilon S_k \frac{\varepsilon}{k}$$

The following source term is added to the transport equation for the specific dissipation rate, ω:

$$\alpha_\omega S_k \frac{\omega}{k}$$

Suitable values for the model parameters C_k, C_ε, and α_ω are not as well established as the parameters for single-phase flow. In the literature, values within the ranges $0.01 < C_k < 1$, $1 < C_\varepsilon < 1.92$ have been suggested (Ref. 1), and α_ω can be defined as $\alpha_\omega = C_\varepsilon - 1$.

In the v2-f turbulence model, the ζ-equation also gets a contribution,

$$\left(2\frac{|\mathbf{u}_{slip} \cdot \nabla l_w|}{|\mathbf{u}_{slip}| \cdot |\nabla l_w|} - \zeta\right)\frac{S_k}{k}$$

where l_w is the wall distance variable and its gradient gives the wall-normal direction. Such modeling assumes that the bubble-induced turbulence kinetic energy is pumped into the component of k aligned with $\mathbf{u}_{slip}$.

The turbulent viscosity appears in the momentum equation and when adding a drift term to the gas velocity:

$$\mathbf{u}_{drift} = -D_{gc}\frac{\nabla \phi_g}{\phi_g}$$

Using a turbulence model that solves for the turbulent kinetic energy, k, together with a gas concentration that is not assumed to be low, the stress tensor contains an extra contribution, and the momentum equations becomes

$$\begin{aligned}\phi_l \rho_l \frac{\partial \mathbf{u}_l}{\partial t} + \phi_l \rho_l \mathbf{u}_l \cdot \nabla \mathbf{u}_l = \\ = -\nabla p + \nabla \cdot \left[\phi_l(\mu_l + \mu_T)\left(\nabla \mathbf{u}_l + \nabla \mathbf{u}_l^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_l)\mathbf{I}\right) - \frac{2}{3}\phi_l \rho_l k \mathbf{I}\right] + \phi_l \rho_l \mathbf{g} + \mathbf{F}\end{aligned} \tag{6-40}$$

References for the Bubbly Flow Interfaces

1. A. Sokolichin, G. Eigenberger, and A. Lapin, "Simulations of Buoyancy Driven Bubbly Flow: Established Simplifications and Open Questions", *AIChE Journal*, vol. 50, no. 1, pp. 24–49, 2004.

2. D. Kuzmin and S. Turek, *Efficient Numerical Techniques for Flow Simulation in Bubble Column Reactors*, Institute of Applied Mathematics, University of Dortmund, 2000.

3. D. Kuzmin, S. Turek, and H. Haario, *Finite Element Simulation of Turbulent Bubbly Flows in Gas-liquid Reactors*, Ergebnisberichte Angew, Math, 298, University of Dortmund, 2005.

4. M.P. Schwarz and W.J. Turner, "Applicability of the Standard k-ε Turbulence Model to Gas-stirred Baths", *Applied Mathematical Modelling*, vol. 12, pp. 273–279, 1988.

5. C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows with Droplets and Particles*, CRC Press, 1998.

Theory for the Mixture Model Interfaces

The mixture model is a macroscopic two-phase flow model, in many ways similar to the bubbly flow model. It tracks the averaged phase concentration, or volume fraction, and solves a single momentum equation for the mixture velocity. It is suitable for mixtures consisting of solid particles or liquid droplets immersed in a liquid.

The Mixture Model interface theory is described in this section:

- The Mixture Model Equations
- Dispersed Phase Boundary Condition Equations
- Turbulence Modeling in Mixture Models
- Slip Velocity Models
- References for the Mixture Model Interfaces

The Mixture Model Equations

In the Mixture Model interfaces the particle-fluid combination is regarded as a single flowing continuum with macroscopic properties such as density and viscosity. The two phases consist of one dispersed phase and one continuous phase. The mixture model is valid if the continuous phase is a liquid, and the dispersed phase consists of solid particles, liquid droplets, or gas bubbles. For gas bubbles in a liquid, however, the bubbly flow model is preferable. The mixture model relies on the following assumptions:

- The density of each phase is approximately constant.
- Both phases share the same pressure field.
- The particle relaxation time is short compared to the time-scales of the macroscopic flow.

The mixture density is given by

$$\rho = \phi_c \rho_c + \phi_d \rho_d$$

where

- ϕ_c and ϕ_d denote the volume fractions of the continuous phase and the dispersed phase (SI unit: m^3/m^3), respectively
- ρ_c is the continuous phase density (SI unit: kg/m^3), and
- ρ_d is the dispersed phase density (SI unit: kg/m^3).

The volume flux for each phase is

$$\mathbf{j}_d = \phi_d \mathbf{u}_d$$

$$\mathbf{j}_c = \phi_c \mathbf{u}_c$$

where $\mathbf{u}_c$ and $\mathbf{u}_d$ (SI unit: m/s) are the continuous and the dispersed phase velocity vectors, respectively.

In previous versions of COMSOL Multiphysics (prior to version 5.4, see Mass-Averaged Mixture Velocity), the mixture velocity used was the mass-averaged mixture velocity $\mathbf{u}$ (SI unit: m/s), defined as

$$\mathbf{u} = \frac{\phi_c \rho_c \mathbf{u}_c + \phi_d \rho_d \mathbf{u}_d}{\rho} \tag{6-41}$$

The mixture velocity used here is the volume-averaged flux density, or volume-averaged mixture velocity $\mathbf{j}$ (SI unit: m/s), defined as

$$\mathbf{j} = \mathbf{j}_d + \mathbf{j}_c$$

The continuity equation for the mixture is

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{6-42}$$

In the Mixture Model interfaces it is assumed that the densities of both phases, ρ_c and ρ_d, are constant, and therefore the following alternative form of the continuity equation for the mixture is used

$$\nabla \cdot \mathbf{j} = m_{dc}\left(\frac{1}{\rho_c} - \frac{1}{\rho_d}\right) \tag{6-43}$$

The momentum equation for the mixture is

$$\rho \mathbf{j}_t + \rho(\mathbf{j} \cdot \nabla)\mathbf{j} + \rho_c \varepsilon(\mathbf{j}_{slip} \cdot \nabla)\mathbf{j} = -\nabla p + \nabla \cdot \tau_{Gm} + \rho \mathbf{g} + \mathbf{F}$$
$$-\nabla \cdot [\rho_c(1 + \phi_c \varepsilon)\mathbf{u}_{slip}\mathbf{j}_{slip}{}^T]$$
$$-\rho_c \varepsilon \left[(\mathbf{j} \cdot \nabla)\mathbf{j}_{slip} + (\nabla \cdot (D_{md} \nabla \phi_d))\mathbf{j} + \mathbf{j}_{slip} m_{dc}\left(\frac{1}{\rho_c} - \frac{1}{\rho_d}\right)\right]$$

where:

- $\mathbf{j}$ is the velocity vector (SI unit: m/s)
- ρ is the density (SI unit: kg/m^3)
- p is the pressure (SI unit: Pa)
- ε is the reduced density difference (SI unit: kg/kg)
- $\mathbf{u}_{slip}$ is the slip velocity vector between the two phases (SI unit: m/s)
- $\mathbf{j}_{slip}$ is the slip flux (SI unit: m/s)
- τ_{Gm} is the sum of the viscous and turbulent stresses (SI unit: kg/(m·s^2))
- D_{md} is a turbulent dispersion coefficient (SI unit: m^2/s)
- m_{dc} is the mass transfer rate from the dispersed to the continuous phase (SI unit: kg/(m^3·s))
- $\mathbf{g}$ is the gravity vector (SI unit: m/s^2), and
- $\mathbf{F}$ is any additional volume force (SI unit: N/m^3)

The slip flux is defined for convenience as,

$$\mathbf{j}_{slip} = \phi_d \phi_c \mathbf{u}_{slip} \tag{6-44}$$

Here, $\mathbf{u}_{slip}$ (SI unit: m/s) denotes the relative velocity between the two phases. For different available models for the slip velocity, see Slip Velocity Models.

The reduced density difference ε is given by

$$\varepsilon = \frac{\rho_d - \rho_c}{\rho_c}$$

The sum of the viscous and turbulent stresses is

$$\tau_{Gm} = (\mu + \mu_T)[\nabla \mathbf{j} + \nabla \mathbf{j}^T] - \frac{2}{3}(\mu + \mu_T)(\nabla \cdot \mathbf{j})\mathbf{I} - \frac{2}{3}\rho k \mathbf{I} \tag{6-45}$$

where μ (SI unit: Pa·s) is the mixture viscosity, μ_T (SI unit: Pa·s) the turbulent viscosity, and k (SI unit: m^2/s^2) is the turbulent kinetic energy, when available. If no turbulence model is used, μ_T and k equal zero

The transport equation for ϕ_d, the dispersed phase volume fraction, is

$$\frac{\partial}{\partial t}(\phi_d \rho_d) + \nabla \cdot (\phi_d \rho_d \mathbf{u}_d) = \nabla \cdot (\rho_d D_{md} \nabla \phi_d) - m_{dc} \tag{6-46}$$

where m_{dc} (SI unit: $kg/(m^3 \cdot s)$) is the mass transfer rate from the dispersed to the continuous phase and D_{md} is a turbulent dispersion coefficient (SI unit: m^2/s) (see Turbulence Modeling in Mixture Models), accounting for extra diffusion due to turbulent eddies. When a turbulence model is not used, D_{md} is zero. Assuming constant density for the dispersed phase and using Equation 6-43, Equation 6-46 can be rewritten as

$$\frac{\partial}{\partial t}(\phi_d) + \mathbf{j} \cdot \nabla \phi_d + \nabla \cdot (\mathbf{j}_{slip}) = \nabla \cdot (D_{md} \nabla \phi_d) - \frac{m_{dc} \rho}{\rho_d \rho_c} \tag{6-47}$$

The continuous phase volume fraction ϕ_c is

$$\phi_c = 1 - \phi_d$$

MASS TRANSFER AND INTERFACIAL AREA

It is possible to account for mass transfer between the two phases by specifying an expression for the mass transfer rate from the dispersed phase to the continuous m_{dc} (SI unit: $kg/(m^3 \cdot s)$).

The mass transfer rate typically depends on the interfacial area between the two phases. An example is when gas dissolves into a liquid. In order to determine the interfacial area, it is necessary to solve for the dispersed phase number density (that is, the number of particles per volume) in addition to the phase volume fraction. The Mixture Model interface assumes that the particles can increase or decrease in size but not completely vanish, merge, or split. The conservation of the number density n (SI unit: $1/m^3$) then gives

$$\frac{\partial n}{\partial t} + \mathbf{j} \cdot \nabla n + \nabla \cdot (n \phi_c \mathbf{u}_{slip}) = \nabla \cdot (D_{md} \nabla n) - n m_{dc} \left(\frac{1}{\rho_c} - \frac{1}{\rho_d} \right)$$

The number density and the volume fraction dispersed particles give the interfacial area per unit volume (SI unit: m^2/m^3):

$$a = (4n\pi)^{1/3}(3\phi_d)^{2/3}$$

MASS-AVERAGED MIXTURE VELOCITY

In previous versions of COMSOL Multiphysics (prior to version 5.4), the mixture velocity used was the mass-averaged mixture velocity $\mathbf{u}$ (SI unit: m/s), see Equation 6-41. The continuity equation was

$$(\rho_c - \rho_d)\left[\nabla \cdot (\phi_d(1-c_d)\mathbf{u}_{slip} - D_{md}\nabla\phi_d) + \frac{m_{dc}}{\rho_d}\right] + \rho_c(\nabla \cdot \mathbf{u}) = 0 \qquad (6\text{-}48)$$

and the transport equation for ϕ_d was

$$\frac{\partial}{\partial t}(\phi_d) + \nabla \cdot (\phi_d \mathbf{u}_d) = \nabla \cdot (D_{md}\nabla\phi_d) - \frac{m_{dc}}{\rho_d} \qquad (6\text{-}49)$$

The dispersed phase velocity vector $\mathbf{u}_d$ and the mass fraction of the dispersed phase c_d are given by

$$\mathbf{u}_d = \mathbf{u} + (1-c_d)\mathbf{u}_{slip}$$

$$c_d = \frac{\phi_d \rho_d}{\rho}$$

The continuity equation Equation 6-48 is incompatible with the no-penetration condition of $\mathbf{u}$ at the walls, and $\mathbf{u}$ is not divergence-free. The volume-averaged velocity $\mathbf{j}$ is solenoidal and Equation 6-43 is compatible with the no-penetration condition at the walls (as long as there is no mass transfer or the densities of the two phases are equal).

Dispersed Phase Boundary Condition Equations

In addition to the boundary conditions for the mixture, specify boundary conditions for the dispersed phase on Wall, Inlet, and Outlet nodes. For these boundary types, the boundary condition's Settings window contains a Dispersed Phase Boundary Condition section.

DISPERSED PHASE CONCENTRATION

This is the default for the Inlet node. Specify the dispersed phase volume fraction:

$$\phi_d = \phi_{d0}$$

Enter the **Dispersed phase volume fraction** (dimensionless) in the ϕ_{d0} field.

If **Solve for interfacial area** is selected under the **Physical Model** section, the dispersed phase number density is also specified. The dispersed phase number density can be specified directly,

$$n = n_0$$

or, when **Diameter of particles/droplets** is selected, computed from the diameter of particles and droplets d_d:

$$n = 6\frac{\phi_{d0}}{\pi d_d^3}$$

DISPERSED PHASE OUTLET

This is the default for the Outlet node. This boundary condition is appropriate for boundaries where the dispersed phase leaves the domain with the dispersed phase velocity $\mathbf{u}_d$. No condition is imposed on the volume fractions at the boundary.

A corresponding flux condition is also applied for the number density equation (when **Solve for interfacial area** is selected under the **Physical Model** section).

DISPERSED PHASE FLUX

Using this boundary condition, specify the dispersed phase flux through the boundary:

$$-\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = N_{\phi_d}$$

Enter the **Dispersed phase flux** (SI unit: m/s) in the N_{ϕ_d} field.

If **Solve for interfacial area** is selected under the **Physical Model** section, the number density flux through the boundary is also specified:

$$-\mathbf{n} \cdot (n\mathbf{u}_d) = N_{n_d}$$

SYMMETRY

This boundary condition, which is useful on boundaries that represent a symmetry line for the dispersed phase, sets the dispersed phase flux through the boundary to zero:

$$\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = 0$$

A corresponding flux condition is also applied for the number density equation (when **Solve for interfacial area** is selected under the **Physical Model** section).

NO DISPERSED FLUX

This is the default for the Wall node. This boundary condition represents boundaries where the dispersed phase flux through the boundary is zero:

$$\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = 0$$

In the case of moving Wall and Interior Wall, the dispersed flux through the boundary is:

$$\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = \mathbf{n} \cdot (\phi_d \mathbf{j})$$

This implies that the flux, relative to the boundary motion, is zero. A corresponding flux condition is also applied for the number density equation (when **Solve for interfacial area** is selected under the **Physical Model** section).

Turbulence Modeling in Mixture Models

Turbulence modeling is particularly relevant for dilute flows, that is, for flows with a low dispersed phase volume fraction. For dense flows, the mixture viscosity usually becomes high. In such cases, the flow is laminar and no turbulence modeling is necessary.

The Mixture Model, Turbulent Flow interfaces include the turbulence models described in Theory for the Turbulent Flow Interfaces.

The turbulence must be accounted for in the calculation of the dispersed phase volume fraction. This is accomplished by introducing a turbulent dispersion coefficient D_{md} (SI unit: m^2/s) in Equation 6-47 as

$$D_{md} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is the turbulent particle Schmidt number (dimensionless). The particle Schmidt number is usually suggested as a value ranging from 0.35 to 0.7. In the physics interface the default value is 0.35. The so-called drift velocity is included in Equation 6-47 as a diffusion term

$$\frac{\partial}{\partial t}(\phi_d) + \mathbf{j} \cdot \nabla \phi_d + \nabla \cdot (\mathbf{j}_{slip}) = \nabla \cdot (D_{md} \nabla \phi_d) - \frac{m_{dc} \rho}{\rho_d \rho_c}$$

Similarly, the number density equation (used to compute the interfacial area) for turbulent flow corresponds to

$$\frac{\partial n}{\partial t} + \mathbf{j} \cdot \nabla n + \nabla \cdot (n\phi_c \mathbf{u}_{\text{slip}}) = \nabla \cdot (D_{m\text{d}} \nabla n) - n m_{\text{dc}} \left(\frac{1}{\rho_c} - \frac{1}{\rho_{\text{d}}} \right)$$

The inclusion of the drift velocity in Equation 6-47 modifies the flux of the dispersed phase. The effective dispersed phase flux $\mathbf{j}_{\text{d,eff}}$ and velocity $\mathbf{u}_{\text{d,eff}}$ are given by

$$\mathbf{j}_{\text{d, eff}} = \mathbf{j}_{\text{d}} - D_{m\text{d}} \nabla \phi_{\text{d}}$$

$$\mathbf{u}_{\text{d, eff}} = \mathbf{u}_{\text{d}} - \frac{D_{m\text{d}}}{\phi_{\text{d}}} \nabla \phi_{\text{d}}$$

$\mathbf{j}_{\text{d,eff}}$ and $\mathbf{u}_{\text{d,eff}}$ are available in the physics interface as `mm.jdEff` and `mm.udEff`.

Slip Velocity Models

The Mixture Model interfaces contain three predefined models for the relative velocity between the two phases $\mathbf{u}_{\text{slip}}$ (SI unit: m/s):

- The *Schiller–Naumann model*
- The *Haider–Levenspiel model*
- The *Hadamard–Rybczynski model*

All three models use the following relation for the slip velocity:

$$\frac{3}{4} \frac{C_{\text{d}}}{d_{\text{d}}} |\mathbf{u}_{\text{slip}}| \mathbf{u}_{\text{slip}} = -\frac{(\rho - \rho_{\text{d}})}{\rho_c} \left(-\mathbf{j}_t - (\mathbf{j} \cdot \nabla)\mathbf{j} + \mathbf{g} + \frac{\mathbf{F}}{\rho} \right) \quad (6\text{-}50)$$

where C_{d} (dimensionless) is the particle drag coefficient. Essentially, interpret the relation as a balance between viscous drag and buoyancy forces acting on the dispersed phase.

The Schiller–Naumann model models the drag coefficient according to

$$C_{\text{d}} = \begin{cases} \frac{24}{\text{Re}_{\text{p}}} (1 + 0{,}15 \text{Re}_{\text{p}}^{0{,}687}) & \text{Re}_{\text{p}} < 1000 \\ 0{,}44 & \text{Re}_{\text{p}} > 1000 \end{cases}$$

where Re_{p} is the particle Reynolds number

$$\text{Re}_{\text{p}} = \frac{d_{\text{d}} \rho_c |\mathbf{u}_{\text{slip}}|}{\mu}$$

Note that this definition of the particle Reynolds number uses the viscosity of the mixture and not the viscosity of the continuous phase, as would be customary for a single particle in a pure fluid with viscosity μ_c. This choice incorporates the hindrance effect of the other particles on the slip velocity, see Ref. 4.

Because the particle Reynolds number depends on the slip velocity, an implicit equation must be solved to obtain the slip velocity. Therefore, the Mixture Model interfaces add an additional equation for

$$|\mathbf{u}_{\text{slip}}|^2$$

when the Schiller–Naumann slip model is used. The Schiller–Naumann model is particularly well-suited for solid particles in a liquid.

The Haider–Levenspiel model is applicable to nonspherical particles. It models the drag coefficient according to

$$C_d = \frac{24}{\text{Re}_p}\left(1 + A(S_p)\text{Re}_p^{B(S_p)}\right) + \frac{C(S_p)}{1 + D(S_p)/\text{Re}_p}$$

where A, B, C, and D are empirical correlations of the particle sphericity. The sphericity is defined as the ratio of the surface area of a volume equivalent sphere to the surface area of the considered nonspherical particle

$$0 < S_p = \frac{A_{\text{sphere}}}{A_{\text{particle}}} \leq 1$$

The correlation coefficients are given by

$$A(S_p) = e^{2.3288 - 6.4581S_p + 2.4486S_p^2}$$
$$B(S_p) = 0.0964 + 0.5565S_p$$
$$C(S_p) = e^{4.905 - 13.8944S_p + 18.4222S_p^2 - 10.2599S_p^3}$$
$$D(S_p) = e^{1.4681 + 12.2584S_p - 20.7322S_p^2 + 15.8855S_p^3}$$

The diameter used in the particle Reynolds number is that of the volume equivalent sphere. The equation for the squared slip velocity is also added when the Haider–Levenspiel slip model is used.

The Hadamard–Rybczynski drag law is valid for particle Reynolds numbers less than 1, for particles, bubbles, and droplets. The drag coefficient for liquid droplets or bubbles is

$$C_d = \frac{24}{Re_p}\left(\frac{1+\frac{2}{3}\frac{\mu_c}{\mu_d}}{1+\frac{\mu_c}{\mu_d}}\right)$$

which yields the following explicit expression for the slip velocity

$$\mathbf{u}_{slip} = -\frac{(\rho-\rho_d)d_d^2}{18\mu}\left(\frac{1+\frac{\mu_c}{\mu_d}}{1+\frac{2}{3}\frac{\mu_c}{\mu_d}}\right)\left(-\mathbf{j}_t-(\mathbf{j}\cdot\nabla)\mathbf{j}+\mathbf{g}+\frac{\mathbf{F}}{\rho}\right)$$

For solid particles, the slip velocity is given by

$$\mathbf{u}_{slip} = -\frac{(\rho-\rho_d)d_d^2}{18\mu}\left(-\mathbf{j}_t-(\mathbf{j}\cdot\nabla)\mathbf{j}+\mathbf{g}+\frac{\mathbf{F}}{\rho}\right)$$

when $Re_p < 1$. For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

References for the Mixture Model Interfaces

1. M. Manninen, V. Taivassalo, and S. Kallio, *On the Mixture Model for Multiphase Flow,* VTT Publications, 288, VTT Energy, Nuclear Energy, Technical Research Center of Finland (VTT), 1996.

2. C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows with Droplets and Particles,* CRC Press, 1998.

3. M.S. Nigam, "Numerical Simulation of Buoyant Mixture Flows," *Int. Jour. of Multi. Flow.*, vol. 29, pp. 983–1015, 2003.

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Theory for the Euler–Euler Model Interfaces

The Euler–Euler Model interfaces are based on averaging the Navier–Stokes equations for each present phase over a volume that is small compared to the computational domain but large compared to the dispersed phase (particles, droplets, or bubbles). The two phases, the continuous and the dispersed phase, are assumed to behave as two continuous and interpenetrating fluids, and the physics interface solves one set of momentum equations for each phase.

In this section:

- The Euler–Euler Model Equations
- Some Notes on Boundary Conditions
- Turbulent Two-Phase Flow Modeling
- References for the Euler–Euler Model Interfaces

The Euler–Euler Model Equations

MASS BALANCE

The following continuity relations hold for the continuous and dispersed phases (Ref. 3):

$$\frac{\partial}{\partial t}(\rho_c \phi_c) + \nabla \cdot (\rho_c \phi_c \mathbf{u}_c) = m_{dc} \tag{6-51}$$

$$\frac{\partial}{\partial t}(\rho_d \phi_d) + \nabla \cdot (\rho_d \phi_d \mathbf{u}_d) = -m_{dc} \tag{6-52}$$

Here ϕ (dimensionless) denotes the phase volume fraction, ρ (SI unit: kg/m^3) is the density, $\mathbf{u}$ (SI unit: m/s) the velocity of each phase, and m_{dc} is the mass transfer rate from the dispersed to the continuous phase (SI unit: $kg/(m^3 \cdot s)$). The subscripts c and d denote quantities relating to the continuous and the dispersed and phase, respectively. The following relation between the volume fractions must hold

$$\phi_c = 1 - \phi_d$$

Both phases are considered to be incompressible, in which case Equation 6-51 and Equation 6-52 can be simplified as:

$$\frac{\partial \phi_c}{\partial t} + \nabla \cdot (\phi_c \mathbf{u}_c) = \frac{m_{dc}}{\rho_c} \tag{6-53}$$

$$\frac{\partial \phi_d}{\partial t} + \nabla \cdot (\phi_d \mathbf{u}_d) = -\frac{m_{dc}}{\rho_d} \tag{6-54}$$

If Equation 6-54 and Equation 6-53 are added together, a continuity equation for the mixture is obtained:

$$\nabla \cdot (\phi_d \mathbf{u}_d + \mathbf{u}_c(1-\phi_d)) = m_{dc}\left(\frac{1}{\rho_c} - \frac{1}{\rho_d}\right) \tag{6-55}$$

In order to control the mass balance of the two phases, the Euler–Euler Model interfaces solves Equation 6-54 together with Equation 6-55. Equation 6-54 is used to compute the volume fraction of the dispersed phase, and Equation 6-55 is used to compute the mixture pressure.

MOMENTUM BALANCE

The momentum equations for the continuous and dispersed phases, using the nonconservative forms (see for example Ref. 3 or Ref. 9), are:

$$\rho_c \phi_c \left[\frac{\partial}{\partial t}(\mathbf{u}_c) + \mathbf{u}_c \nabla \cdot (\mathbf{u}_c)\right] = -\phi_c \nabla p + \phi_c \nabla \cdot \tau_c + \phi_c \rho_c \mathbf{g} + \mathbf{F}_{m,c} + \phi_c \mathbf{F}_c + m_{dc}(\mathbf{u}_{int} - \mathbf{u}_c) \tag{6-56}$$

$$\rho_d \phi_d \left[\frac{\partial}{\partial t}(\mathbf{u}_d) + \mathbf{u}_d \nabla \cdot (\mathbf{u}_d)\right] = -\phi_d \nabla p + \phi_d \nabla \cdot \tau_d + \phi_d \rho_d \mathbf{g} + \mathbf{F}_{m,d} + \phi_d \mathbf{F}_d - m_{dc}(\mathbf{u}_{int} - \mathbf{u}_d) \tag{6-57}$$

Here p (SI unit: Pa) is the mixture pressure, which is assumed to be equal for the two phases. In the momentum equations the viscous stress tensor for each phase is denoted by τ (SI unit: Pa), $\mathbf{g}$ (SI unit: m/s^2) is the vector of gravitational acceleration, $\mathbf{F}_m$ (SI unit: N/m^3) is the interphase momentum transfer term (that is, the volume force exerted on each phase by the other phase), $\mathbf{F}$ (SI unit: N/m^3) is any other volume force term, and $\mathbf{u}_{int}$ is the interphase velocity (SI unit: m/s).

In these equations, the influence of surface tension in the case of liquid phases has been neglected, and the potential size distribution of the dispersed particles or droplets is not considered.

For fluid-solid mixtures where $\rho_d >> \rho_c$, Equation 6-57 is modified in the manner of Enwald (Ref. 5)

$$\rho_d \phi_d \left[\frac{\partial}{\partial t}(\mathbf{u}_d) + \mathbf{u}_d \nabla \cdot (\mathbf{u}_d) \right] = \\ -\phi_d \nabla p - \nabla p_s + \phi_d \rho_d \mathbf{g} + \mathbf{F}_{m,d} + \phi_d \mathbf{F}_d - m_{dc}(\mathbf{u}_{int} - \mathbf{u}_d) \tag{6-58}$$

where p_s (SI unit: Pa) is the solid pressure.

The fluid phases in the above equations are assumed to be Newtonian and the viscous stress tensors are defined as

$$\tau_c = \mu_c^m \left(\nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_c)\mathbf{I} \right)$$

$$\tau_d = \mu_d^m \left(\nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_d)\mathbf{I} \right)$$

where μ_c^m and μ_d^m (SI unit: Pa·s) are the dynamic viscosity model of the respective phase. Observe how the viscous terms in equation Equation 6-56 and Equation 6-57 appear with their volume fractions outside the divergence operators. The equations can also be derived so that the terms read $\nabla \cdot (\phi_c \tau_c)$ and $\nabla \cdot (\phi_d \tau_d)$ instead (see for example Ref. 4 or Ref. 5). It depends on exactly how the derivation is carried out. formulation in Equation 6-56 and Equation 6-57 are so that the momentum equation can be divided by ϕ_c and ϕ_d, respectively as described below.

In order to avoid singular solutions when the volume fractions tend to zero, the governing equations above are divided by the corresponding volume fraction. The implemented momentum equation for the continuous phase is:

$$\rho_c \frac{\partial}{\partial t}(\mathbf{u}_c) + \rho_c \mathbf{u}_c \nabla \cdot (\mathbf{u}_c) = -\nabla p + \nabla \cdot \tau_c + \rho_c \mathbf{g} + \frac{\mathbf{F}_{m,c}}{\phi_c} + \mathbf{F}_c + \frac{m_{dc}}{\phi_c}(\mathbf{u}_{int} - \mathbf{u}_c)$$

The implemented momentum equations for the dispersed phase in the case of dispersed liquid droplets or bubbles is:

$$\rho_d\left[\frac{\partial}{\partial t}(\mathbf{u}_d)+\mathbf{u}_d\nabla\cdot(\mathbf{u}_d)\right]=$$
$$-\nabla p+\nabla\cdot\tau_d+\rho_d\mathbf{g}+\frac{\mathbf{F}_{m,d}}{\phi_d}+\mathbf{F}_d-\frac{m_{dc}}{\phi_d}(\mathbf{u}_{int}-\mathbf{u}_d) \quad (6\text{-}59)$$

and in the case of dispersed solid particles:

$$\rho_d\left[\frac{\partial}{\partial t}(\mathbf{u}_d)+\mathbf{u}_d\nabla\cdot(\mathbf{u}_d)\right]=$$
$$-\nabla p-\frac{\nabla p_s}{\phi_d}+\rho_d\mathbf{g}+\frac{\mathbf{F}_{m,d}}{\phi_d}+\mathbf{F}_d-\frac{m_{dc}}{\phi_d}(\mathbf{u}_{int}-\mathbf{u}_d) \quad (6\text{-}60)$$

VISCOSITY MODELS

The Newtonian viscosities of interpenetrating media are not readily available. Instead empirical and analytical models for the dynamic viscosity of the two-phase mixture have been developed by various researchers, usually as a function of the dispersed volume fraction. Using an expression for the mixture viscosity, the default values for the dynamic viscosities of the two interpenetrating phases are taken to be:

$$\mu_c^m=\mu_d^m=\mu_{mix} \quad (6\text{-}61)$$

A simple mixture viscosity covering the entire range of particle concentrations is the Krieger type model (Ref. 5):

$$\mu_{mix}=\mu_c\left(1-\frac{\phi_d}{\phi_{d,max}}\right)^{-2.5\phi_{d,max}} \quad (6\text{-}62)$$

Here $\phi_{d,max}$ is the maximum packing limit, by default 0.62 for solid particles. Equation 6-62 can be applied when $\mu_c \ll \mu_d$. An extension of Equation 6-62 can be applied for liquid droplets/bubbles:

$$\mu_{mix}=\mu_c\left(1-\frac{\phi_d}{\phi_{d,max}}\right)^{-2.5\phi_{d,max}\frac{\mu_d+0.4\mu_c}{\mu_d+\mu_c}} \quad (6\text{-}63)$$

For liquid droplets/bubbles the default value of $\phi_{d,max}$ is 1.

For fluid-fluid systems, the simple relation

$$\mu_{mix}=\phi_c\mu_c+\phi_d\mu_d \quad (6\text{-}64)$$

can sometimes be applied or the viscosity for each individual phase can be applied to the respective momentum equation.

An alternative to mixture viscosity for dispersed solid particles, that is particles in gas flow, is to model the particle interface with a solid pressure instead (see Solid Pressure). A small viscosity is however necessary for numerical robustness and Gidaspow (Ref. 6) suggested to use

$$\mu_d^m = 0.5\max(\phi_d, \phi_{d,res}) \tag{6-65}$$

This is consistent with the requirement that $\mu_d^m \to 0$ when $\phi_d \to 0$ (Ref. 9), but in practice it can suffice with any small enough, nonzero value.

INTERPHASE MOMENTUM TRANSFER

In all the equations, $\mathbf{F}_m$ denotes the interphase momentum transfer, that is the force imposed on one phase by the other phase. Considering a particle, droplet, or bubble in a fluid flow, it is affected by a number of forces, for example, the drag force, the added mass force, the Basset force, and the lift force. The most important force is usually the drag force, especially in fluids with a high concentration of dispersed solids, and hence this is the predefined force included in the Euler–Euler model. The drag force added to the momentum equation is defined as:

$$\mathbf{F}_{drag,c} = -\dot{\mathbf{F}}_{drag,d} = \beta \mathbf{u}_{slip} \tag{6-66}$$

where β is a drag force coefficient and the slip velocity is defined as

$$\mathbf{u}_{slip} = \mathbf{u}_d - \mathbf{u}_c$$

The drag force on the dispersed phase is equal to the one on the continuous phase but is working in the opposite direction.

The drag force coefficient, β, is for solid particles often written as (Ref. 2)

$$\beta = \frac{3}{4d_d}\phi_d C_D \rho_c |\mathbf{u}_{slip}| \tag{6-67}$$

For fluid-fluid system, Equation 6-67 is regularized to read (Ref. 12)

$$\beta = \frac{3}{4d_d}\phi_d \phi_c C_D \rho_c |\mathbf{u}_{slip}| \tag{6-68}$$

which is consistent with a vanishing β if $\phi_c \to 0$. All drag force models except Gidaspow are based on Equation 6-67 for solid particles and on Equation 6-68 for bubbles and droplets.

Gidaspow

For dense particle flows with a high concentration of the dispersed phase — for example, in fluidized bed models — the Gidaspow model (Ref. 6) for the drag coefficient can be used. It combines the Wen and Yu (Ref. 7) fluidized state expression:

For $\phi_c > 0.8$

$$\beta = \frac{3\phi_c\phi_d\rho_c C_d}{4d_d}|\mathbf{u}_{slip}|\phi_c^{-2.65} \tag{6-69}$$

with the Ergun (Ref. 8) packed bed expression:

For $\phi_c < 0.8$

$$\beta = 150\frac{\mu_c\phi_d^2}{\phi_c d_d^2} + 1.75\frac{\phi_d\rho_c}{d_d}|\mathbf{u}_{slip}| \tag{6-70}$$

In the above equations, d_d (SI unit: m) is the dispersed particle diameter, and C_d is the drag coefficient for a single dispersed particle. The drag coefficient is in general a function of the particle Reynolds number

$$\mathrm{Re}_p = \frac{d_d\rho_c|\mathbf{u}_{slip}|}{\mu_c}$$

No universally valid expression for the drag coefficient exists. Using the implemented Gidaspow model, C_d is computed using the Schiller–Naumann relation.

Schiller–Naumann

The Schiller–Naumann model describes the drag coefficient in Equation 6-67 and Equation 6-68 for a single rigid sphere (see for example Ref. 3)

$$C_d = \begin{cases} \frac{24}{\mathrm{Re}_p}(1 + 0.15\mathrm{Re}_p^{0.687}) & \mathrm{Re}_p < 1000 \\ 0.44 & \mathrm{Re}_p > 1000 \end{cases} \tag{6-71}$$

It is valid for particle Reynolds numbers up to some critical Reynolds number, approximately equal to $2.5 \cdot 10^5$ where drag crisis occurs.

The Schiller–Naumann model is appropriate for diluted flows since the correlation in Equation 6-71 is based on a single particle and does not take particle-particle interaction into account.

The Schiller–Naumann model can be applied to small fluid particles since they do not deform significantly.

Hadamard–Rybczynski

The Hadamard–Rybczynski drag law is valid for dilute flows with particle Reynolds number less than one for particles, bubbles, and droplets and is defined as:

$$C_\mathrm{d} = \frac{24}{\mathrm{Re}_\mathrm{p}}\left(\frac{1+\frac{2}{3}\frac{\mu_c}{\mu_d}}{1+\frac{\mu_c}{\mu_d}}\right)$$

for bubbles and droplets and as

$$C_\mathrm{d} = \frac{24}{\mathrm{Re}_\mathrm{p}}$$

for solid particles (the Stokes limit). For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

Ishii–Zuber

The Ishii–Zuber model (Ref. 10) can for solid particles be regarded as a generalization of the Schiller–Naumann model. For solid particles it can be formulated as

$$C_\mathrm{D} = \max\left(\frac{24}{\mathrm{Re}_\mathrm{m}}[1+0.1\mathrm{Re}_\mathrm{m}^{0.75}], 0.45\left[\frac{1+17.67f(\phi_\mathrm{d})^{6/7}}{18.67f(\phi_\mathrm{d})}\right]\right) \tag{6-72}$$

where

$$f(\phi_\mathrm{d}) = \sqrt{\phi_\mathrm{c}}(\mu_\mathrm{c}/\mu_\mathrm{m}) \tag{6-73}$$

and Re_m is a Reynolds number based on the mixture viscosity

$$\mathrm{Re}_\mathrm{m} = \frac{d_\mathrm{d}\rho_c|\mathbf{u}_\mathrm{slip}|}{\mu_\mathrm{m}} \tag{6-74}$$

The Ishii–Zuber model is formulated with the assumption that μ_m is described by a Krieger type model (Equation 6-62 for solids or Equation 6-63 for droplets and bubbles). The dependence on μ_m means that the Ishii–Zuber model is valid also for dense suspensions.

For bubbles and droplets, Ishii and Zuber identify three regimes. At low Reynolds numbers, bubbles and droplets behave in the same way as solid particles and the drag coefficient can be described by

$$C_{D,\,visc} = \frac{24}{Re_m}[1 + 0.1Re_m^{0.75}] \tag{6-75}$$

When the Reynolds number becomes higher, bubbles and droplets start to deform in such a way that the drag coefficient increases linearly with diameter but is independent of viscosity. Ishii and Zuber refer to this as the distorted particle regime and suggest the following correlation for this regime:

$$C_{D,\,dist} = \frac{2}{3}\sqrt{Eo}\left[\frac{1 + 17.67f(\phi_d)^{6/7}}{18.67f(\phi_d)}\right] \tag{6-76}$$

where Eo is the Eötvös number

$$Eo = \frac{g|\rho_c - \rho_d|d_d^2}{\sigma} \tag{6-77}$$

where in turn g is the gravitational constant and σ is the surface tension coefficient. The Eötvös number relates surface tension forces to gravitational forces. The second, "distorted" regime ends when hydrodynamic instabilities prevents the drag from increasing further and the distorted regime is capped by the following value:

$$C_{D,\,cap} = \frac{8}{3}\phi_c^2 \tag{6-78}$$

The complete model for bubbles and droplets can hence be written:

$$C_D = \begin{cases} C_{D,\,visc} & \text{if } C_{D,\,visc} \geq C_{D,\,dist} \\ \min(C_{D,\,dist}, C_{D,\,cap}) & \text{if } C_{D,\,visc} < C_{D,\,dist} \end{cases} \tag{6-79}$$

Haider–Levenspiel

The Haider–Levenspiel model is applicable to dilute flows with nonspherical solid particles. It models the drag coefficient according to

$$C_d = \frac{24}{\mathrm{Re}_p}\left(1 + A(S_p)\mathrm{Re}_p^{B(S_p)}\right) + \frac{C(S_p)}{1 + D(S_p)/\mathrm{Re}_p}$$

where A, B, C, and D are empirical correlations of the particle sphericity (see Slip Velocity Models for further details).

Tomiyama and Others

Tomiyama and others (Ref. 11) provided three correlations for diluted bubbles and droplets. The correlation for purified fluids read

$$C_D = \max\left\{\min\left[\frac{16}{\mathrm{Re}_p}(1 + 0.15\mathrm{Re}_p^{0.687}), \frac{48}{\mathrm{Re}_p}\right], \frac{8}{3}\frac{\mathrm{Eo}}{\mathrm{Eo} + 4}\right\} \tag{6-80}$$

Fluid pure enough for Equation 6-80 to be valid is typically only achievable in laboratory environments. Even small amounts of surface-active impurities can collect at the droplet/bubble interface and cause a surface tension gradient which resists surface movement. The correlation for slightly contaminated fluids therefore prescribe a slightly higher drag coefficient:

$$C_D = \max\left\{\min\left[\frac{24}{\mathrm{Re}_p}(1 + 0.15\mathrm{Re}_p^{0.687}), \frac{72}{\mathrm{Re}_p}\right], \frac{8}{3}\frac{\mathrm{Eo}}{\mathrm{Eo} + 4}\right\} \tag{6-81}$$

This correlation is the default one and applies to droplets and bubbles in fluids of contamination levels comparable to ordinary tap water.

When the contamination level is high, the impurities effectively prevent all motion within the droplet or bubble and the following correlation is suggested:

$$C_D = \max\left\{\min\frac{24}{\mathrm{Re}_p}(1 + 0.15\mathrm{Re}_p^{0.687}), \frac{8}{3}\frac{\mathrm{Eo}}{\mathrm{Eo} + 4}\right\} \tag{6-82}$$

SOLID PRESSURE

For fluid-solid mixtures where $\rho_d >> \rho_c$, for example solid particles in gas flow, a model for the solid pressure, p_s in Equation 6-60, is needed. The solid pressure models the particle interaction due to collisions and friction between the particles. The solid pressure model implemented uses a gradient diffusion based assumption:

$$\nabla p_s = -G(\phi_c)\nabla\phi_c$$

where the empirical function G can be thought of as a modulus of elasticity or powder modulus. A common form for G is (Ref. 5)

$$G(\phi_c) = 10^{B_1\phi_c + B_2} \tag{6-83}$$

The available predefined models (all defined in Ref. 5) are those of Gidaspow and Ettehadieh,

$$G(\phi_c) = 10^{-8.76\phi_c + 5.43} \tag{6-84}$$

Ettehadieh,

$$G(\phi_c) = 10^{-10.46\phi_c + 6.577} \tag{6-85}$$

and Gidaspow,

$$G(\phi_c) = 10^{-10.5\phi_c + 9.0} \tag{6-86}$$

Observe that the solid pressure term theoretically replaces the stress term in the dispersed phase momentum equation. A small viscosity is however necessary for numerical robustness. The Gidaspow formulation or a small constant value is appropriate. The viscosity for the continuous phase, μ_c^m, can be taken as the single phase value, that is $\mu_c^m = \mu_c$.

NOTES ON THE IMPLEMENTATION

There are several equations with potentially singular terms and expressions such as the term

$$\frac{\mathbf{F}_{m,d}}{\phi_d}$$

in Equation 6-59. Also, ϕ_d is a degree of freedom and can therefore, during computations, obtain unphysical values in small areas. This can, in turn, lead to unphysical values of material properties such as viscosity and density. To avoid these problems, the implementation uses the following regularizations:

- $1/\phi_k$, $k = c,d$ is replaced by $1/\phi_{k,pos}$ where

  $$\phi_{k,\,pos} = \max(\phi_k, \phi_{k,res})$$

  The residue volume fractions are per default set to 10^{-4} but can be changed in the Advanced Settings section of the interface settings.

- When appropriate, for example when evaluating drag models and mixture viscosities, ϕ_k, $k = c,d$ are replaced by

$$\phi_{k,\,reg} = \min(\max(\phi_k, 0), 1)$$

  Note however that the continuity equation, Equation 6-55, uses ϕ_k without regularization in order to guarantee mass conservation.

Some Notes on Boundary Conditions

An effect of dividing the momentum equations with ϕ_c and ϕ_d, respectively is that for example $\mathbf{u}_d$ obtains a value even if $\phi_d = 0$. In many cases $\mathbf{u}_d$ will tend to $\mathbf{u}_c$ in lack of a dispersed phase. So on inlets where $\phi_d = 0$, it is appropriate to set $\mathbf{u}_d = \mathbf{u}_c$.

A fixed value for ϕ_d should only be prescribed if there is no transport of ϕ_d toward the inlet. If, for example, a cloud of dispersed phase with higher ϕ_d than the prescribed value somehow reaches the inlet, ϕ_d will actually be "consumed".

When specifying a dispersed phase flux, make sure to specify an appropriate velocity to go with the flux to avoid unphysical concentrations of ϕ_d close to the boundary.

At walls, where it is possible to prescribe a wall leakage, the continuous phase normal velocity is set to

$$\mathbf{u}_c \cdot \mathbf{n} = -\frac{\dot{m}_c}{\rho_c \phi_{c,\,pos}}$$

For a dispersed phase leakage:

$$\mathbf{u}_d \cdot \mathbf{n} = -\frac{\dot{m}_d}{\rho_d \phi_{d,\,pos}}$$

Wall leakage for one phase works best if combined with slip condition for the other phase so that the mixture is given maximum freedom to react to the leakage.

Turbulent Two-Phase Flow Modeling

When the characteristic Reynolds number of the two-phase mixture under investigation becomes high, the flow transitions and becomes turbulent. The influence of the turbulence on the flow characteristics (mixing, particle dispersion, pressure drop, and so on) are usually significant and warrants the use of a turbulence model.

In order to model fluid flow turbulence, the Euler–Euler Model, Turbulent Flow interface uses the k-ε turbulence model. This is realized by solving transport equations for the kinetic energy k (SI unit: m^2/s^2) and the dissipation rate of turbulent kinetic energy ε (SI unit: m^2/s^3).

The interface includes the possibility to model the turbulent flow of the two-phase mixture, or to solve for turbulent flow of each phase separately. In the former case, one set of k-ε equations are solved, while in the latter two sets of k-ε equations are solved for, one for each phase.

MIXTURE TURBULENCE

Mixture turbulence assumes that the turbulence effects on both the continuous and dispersed phase can be modeled by solving for the turbulence of the resulting two-phase mixture. Here this is done using a two-equation k-ε model where the transport of turbulence quantities is based on the mass-averaged mixture velocity

$$\mathbf{u}_m = \frac{\phi_c \rho_c \mathbf{u}_m + \phi_d \rho_d \mathbf{u}_m}{\rho},$$

and a volume-averaged mixture viscosity

$$\mu_m = \phi_c \mu_c^m + \phi_d \mu_d^m$$

This implies that the model is appropriate for flows where the relaxation time of the dispersed particles (the time scale on which particles react to changes in the carrier fluid velocity) is not significantly different to the time scale of the turbulence. It is also appropriate for stratified flows, where the mixture mainly consists of one of the phases.

Setting the **Two-phase turbulence** interface property to **Mixture**, the turbulence of the two-phase flow is modeled by solving the following k and ε equations:

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u}_m \cdot \nabla k = \nabla \cdot \left(\left(\mu_m + \frac{\mu_T}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon \tag{6-87}$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u}_m \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu_m + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} \tag{6-88}$$

The equations correspond to the standard two-equation k-ε model including realizability constraints.

The production term is defined accordingly as

$$P_k = \mu_T\left(\nabla \mathbf{u}_m : (\nabla \mathbf{u}_m + (\nabla \mathbf{u}_m)^T) - \frac{2}{3}(\nabla \cdot \mathbf{u}_m)^2\right) - \frac{2}{3}\rho k \nabla \cdot \mathbf{u}_m$$

and the resulting turbulent viscosity is defined as

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon}$$

where C_μ is a model constant. The viscous stress tensors for the phases are hence defined as

$$\tau_c = (\mu_c^m + \mu_T)\left(\nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_c)\mathbf{I}\right) - \frac{2}{3}\rho_c k \mathbf{I},$$

$$\tau_d = (\mu_d^m + \mu_T)\left(\nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T - \frac{2}{3}(\nabla \cdot \mathbf{u}_d)\mathbf{I}\right) - \frac{2}{3}\rho_d k \mathbf{I}.$$

Assuming mixture turbulence, the transport equation for the volume fraction is:

$$\frac{\partial}{\partial t}(\phi_d) + \nabla \cdot (\phi_d \mathbf{u}_d) = \nabla \cdot (D_{md} \nabla \phi_d) \qquad (6\text{-}89)$$

Here the dispersion of the particulate phase by the turbulent fluctuations is modeled using a gradient based hypothesis. The turbulent dispersion coefficient is defined from the turbulent viscosity of the two-phase mixture in the manner of

$$D_{md} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is a turbulent particle Schmidt number (dimensionless).

The default values of the dimensionless parameters using the Mixture Two-phase turbulence model are:

CONSTANT	VALUE
C_μ	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_k	1.0
σ_ε	1.3
K_v	0.41

CONSTANT	VALUE
B	5.2
σ_T	0.35

PHASE-SPECIFIC TURBULENCE

The phase-specific Two-phase turbulence model assumes that the turbulent flow of the continuous and dispersed phase can be modeled by solving for the turbulence of each phase separately by using two sets of k-ε equations. The model implies that the time scales of the turbulent flow of each phase can differ, but it is also computationally more expensive than assuming solving one set of k-ε equations for the mixture.

Setting the **Two-phase turbulence** interface property to **Phase specific**, the turbulent flow of the two phases is modeled by solving two sets of k and ε equations, one for each phase. For the continuous phase, the transport equations for k and ε are

$$\rho_c \frac{\partial k_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla k_c = \nabla \cdot \left(\left(\mu_c^m + \frac{\mu_{T,c}}{\sigma_{k,c}} \right) \nabla k_c \right) + P_{k,c} - \rho_c \varepsilon_c \tag{6-90}$$

$$\rho_c \frac{\partial \varepsilon_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla \varepsilon_c = \nabla \cdot \left(\left(\mu_c^m + \frac{\mu_{T,c}}{\sigma_{\varepsilon,c}} \right) \nabla \varepsilon_c \right) + C_{\varepsilon 1,c} \frac{\varepsilon_c}{k_c} P_{k,c} - C_{\varepsilon 2,c} \rho \frac{\varepsilon_d^2}{k_d} \tag{6-91}$$

while for the dispersed phase the corresponding equations are

$$\rho_d \frac{\partial k_d}{\partial t} + \rho_d \mathbf{u}_d \cdot \nabla k_d = \nabla \cdot \left(\left(\mu_d^m + \frac{\mu_{T,d}}{\sigma_{k,d}} \right) \nabla k_d \right) + P_{k,d} - \rho_d \varepsilon_d \tag{6-92}$$

$$\rho_d \frac{\partial \varepsilon_d}{\partial t} + \rho_d \mathbf{u}_d \cdot \nabla \varepsilon_d = \nabla \cdot \left(\left(\mu_d^m + \frac{\mu_{T,d}}{\sigma_{\varepsilon,d}} \right) \nabla \varepsilon_d \right) + C_{\varepsilon 1,d} \frac{\varepsilon_d}{k_d} P_{k,d} - C_{\varepsilon 2,d} \rho \frac{\varepsilon_d^2}{k_d} \tag{6-93}$$

The equations for each phase correspond to the standard two-equation k-ε model including realizability constraints.

The production terms are defined as

$$P_{k,c} = \mu_{T,c} \left(\nabla \mathbf{u}_c : (\nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_c)^2 \right) - \frac{2}{3} \rho_c k_d \nabla \cdot \mathbf{u}_c$$

$$P_{k,d} = \mu_{T,d} \left(\nabla \mathbf{u}_d : (\nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_d)^2 \right) - \frac{2}{3} \rho_d k_d \nabla \cdot \mathbf{u}_d$$

The resulting turbulent viscosity, applied individually in the momentum equations of the continuous and the dispersed phases, are

$$\mu_{T,\,c} = \rho_c C_{\mu,\,c}\frac{k_c^2}{\varepsilon_c},\ \mu_{T,\,d} = \rho_d C_{\mu,\,d}\frac{k_d^2}{\varepsilon_d} \tag{6-94}$$

where $C_{\mu,c}$ and $C_{\mu,d}$ are model constants. The viscous stress tensors for the phases are hence defined as

$$\tau_c = (\mu_c^m + \mu_{T,\,c})\left(\nabla\mathbf{u}_c + (\nabla\mathbf{u}_c)^T - \frac{2}{3}(\nabla\cdot\mathbf{u}_c)\mathbf{I}\right) - \frac{2}{3}\rho_c k_c\mathbf{I},$$

$$\tau_d = (\mu_d^m + \mu_{T,\,d})\left(\nabla\mathbf{u}_d + (\nabla\mathbf{u}_d)^T - \frac{2}{3}(\nabla\cdot\mathbf{u}_d)\mathbf{I}\right) - \frac{2}{3}\rho_d k_d\mathbf{I}.$$

As in the case of mixture turbulence, the dispersion of the particulate phase by the turbulent fluctuations is modeled using a gradient based hypothesis (Equation 6-89). For phase-specific turbulence the dispersion coefficient is modeled as a volume average of the respective turbulent diffusivity of each phase

$$D_{m\,d} = \frac{1}{\sigma_{T,\,d}}\left(\phi_c\frac{\mu_{T,\,c}}{\rho_c} + \phi_d\frac{\mu_{T,\,d}}{\rho_d}\right)$$

using a turbulent particle Schmidt number $\sigma_{T,d}$ (dimensionless).

The default values of the turbulence model parameters for phase specific turbulence are

CONTINUOUS PHASE CONSTANTS	VALUE	DISPERSED PHASE CONSTANTS	VALUE
$C_{\mu,c}$	0.09	$C_{\mu,d}$	0.09
$C_{\varepsilon 1,c}$	1.44	$C_{\varepsilon 1,d}$	1.44
$C_{\varepsilon 2,c}$	1.92	$C_{\varepsilon 2,d}$	1.92
$\sigma_{k,c}$	1.0	$\sigma_{k,d}$	1.0
$\sigma_{\varepsilon,c}$	1.3	$\sigma_{\varepsilon,d}$	1.3
$K_{v,c}$	0.41	$K_{v,d}$	0.41
B_c	5.2	B_d	5.2
		$\sigma_{T,d}$	0.35

References for the Euler–Euler Model Interfaces

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Theory for the Phase Transport Interfaces

The **Phase Transport** and **Phase Transport in Porous Media** interfaces are intended for studying the transport of multiple immiscible fluid, gas, or (dispersed) solid phases either in free flow or in flow through a porous medium. The interfaces solve for the averaged volume fractions (also called saturations in a porous medium) of the phases, and does not track the interfaces between the different phases. Both interfaces are based on the macroscopic mass conservation equations of each phase. In a porous medium the effects of the microscopic (or pore scale) interfaces between the phases can be taken into account via the capillary pressure functions.

In this section:

- Phase Transport in Free Flow
- Turbulent Mixing
- Phase Transport in Porous Media
- Predefined Capillary Pressure and Relative Permeability Models
- Porous Medium Discontinuity Boundary Condition
- Free-Porous Interface
- References for the Phase Transport Interfaces

Phase Transport in Free Flow

Suppose the fluid consists of a mixture of $i = 1,\ldots,N$ immiscible phases. The following mass conservation equation describes the transport for an individual phase:

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) = Q_i \tag{6-95}$$

where ρ_i denotes the density (SI unit: kg/m^3), s_i denotes the volume fraction (dimensionless), and $\mathbf{u}_i$ denotes the velocity vector (SI unit: m/s) of phase i. In addition, the term Q_i denotes a mass source for phase i (SI unit: kg/(m^3·s)). It is assumed that the sum of the volume fractions of the phases equals 1:

$$\sum_{i=1}^{N} s_i = 1 \tag{6-96}$$

This means that $N-1$ phase volume fractions are independent and are possible to solve for using Equation 6-124. The volume constraint Equation 6-125 is used to reduce the number of dependent variables: one volume fraction, let us say of phase i_c (to be specified in the main node of the **Phase Transport** interface), is expressed using the other volume fractions:

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i \right) \tag{6-97}$$

Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The **Phase Transport** interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis. In this case it adds a diffusion term proportional to the turbulent kinematic viscosity to the phase transport Equation 6-124, which then becomes

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) - \nabla \cdot \left(\rho_i \frac{\nu_T}{Sc_T} \nabla s_i \right) = Q_i \qquad \text{for} \quad i \neq i_c \tag{6-98}$$

Phase Transport in Porous Media

In a porous domain, the mass conservation equation for each phase is given by:

$$\frac{\partial}{\partial t}(\varepsilon_p \rho_i s_i) + \nabla \cdot (\rho_i \mathbf{u}_i) = Q_i \tag{6-99}$$

Here ε_p (dimensionless) is the porosity, and the vector $\mathbf{u}_i$ should now be interpreted as the volumetric flux of phase i (SI unit $\mathrm{m}^3/(\mathrm{m}^2 \cdot \mathrm{s})$ or $\mathrm{m/s}$). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_i = -\frac{\kappa_{ri}}{\mu_i} \kappa (\nabla p_i - \rho_i \mathbf{g}) \tag{6-100}$$

where κ denotes the permeability (SI unit: m^2) of the porous medium, $\mathbf{g}$ the gravitational acceleration vector (SI unit m/s^2), and μ_i the dynamic viscosity (SI unit: kg/(m·s)), p_i the pressure field (SI unit: Pa), and κ_{ri} the relative permeability (dimensionless) of phase i, respectively.

One phase pressure can be chosen independently, which in the **Phase Transport in Porous Media** interface is chosen to be the phase pressure, p_{i_c}, of the phase computed from the volume constraint, and the other phase pressures are defined by the following $N-1$ capillary pressure relations:

$$p_i = p_{i_c} + p_{c_i}(s_1, \ldots, s_N) \qquad \text{for} \quad i \neq i_c \tag{6-101}$$

Substituting Equation 6-100 into Equation 6-99, and using the volume constraint in Equation 6-125, we arrive at the following $N-1$ equations for the phase volume fractions s_i, $(i \neq i_c)$ that are solved in the **Phase Transport in Porous Media** interface:

$$\frac{\partial}{\partial t}(\varepsilon_p \rho_i s_i) - \nabla \cdot \left(\rho_i \kappa_{ri} \frac{\kappa}{\mu_i}(\nabla(p_{i_c} + p_{c_i}) - \rho_i \mathbf{g})\right) = Q_i \qquad \text{for} \quad i \neq i_c \tag{6-102}$$

The remaining volume fraction is computed from

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i\right) \tag{6-103}$$

Predefined Capillary Pressure and Relative Permeability Models

The capillary pressure functions p_{c_i} can be supplied as user defined expressions, or, in case there are only two phases present in the **Phase Transport in Porous Media** interface, the capillary pressure function can be derived from van Genuchten (Ref. 1) or Brooks and Corey (Ref. 2) models. When either of these predefined models is used, the user has to specify which phase is the wetting phase. If the wetting phase is the same as the phase computed from the volume constraint, then

$$p_i = p_{i_c} + p_{c_i} \qquad \text{for} \quad i \neq i_c \tag{6-104}$$

otherwise

$$p_i = p_{i_c} - p_{c_i} \qquad \text{for} \quad i \neq i_c \tag{6-105}$$

For the van Genuchten model, the expression for the capillary pressure as a function of saturation follows the curve

$$p_c = p_{ec}\left(\frac{1}{(\overline{s_w})^{1/m_{vG}}} - 1\right)^{1-m_{vG}} \tag{6-106}$$

where p_{cc} is the entry capillary pressure and m_{vG} is a constitutive constant, and where $\overline{s_w}$ denotes the effective saturation of the wetting phase. The effective saturation of each phase is defined as

$$\overline{s_i} = (s_i - s_{ri})/\left(1 - \sum_{j=1}^{N} s_{rj}\right) \tag{6-107}$$

where s_{rj} denotes the residual saturation of phase *j*. For the Brooks and Corey model, the capillary pressure curve depends on saturation as

$$p_c = p_{ec}\frac{1}{(\overline{s_w})^{1/\lambda_p}} \tag{6-108}$$

where λ_p is the pore distribution index.

When the van Genuchten or Brooks and Corey capillary pressure model is selected, the relative permeabilities are also determined by these predefined models. For the van Genuchten model, the relative permeabilities are given by

$$\kappa_{rs_w} = (\overline{s_w})^{l_{vG}}\left(1 - (1 - (\overline{s_w})^{1/m_{vG}})^{m_{vG}}\right)^2 \tag{6-109}$$

$$\kappa_{rs_n} = (\overline{s_n})^{l_{vG}}(1 - (1 - \overline{s_n})^{1/m_{vG}})^{2m_{vG}} \tag{6-110}$$

where m_{vG} and l_{vG} are constitutive constants, and where s_n denotes the volume fraction of the nonwetting phase. For the Brooks and Corey model, the relative permeabilities are given by

$$\kappa_{rs_w} = (\overline{s_w})^{(3+2/\lambda_p)} \tag{6-111}$$

$$\kappa_{rs_n} = \overline{s_n}^2(1 - (1 - \overline{s_n})^{(1+2/\lambda_p)}) \tag{6-112}$$

where λ_p is again the pore distribution index.

When for a phase *i* the Power law option is selected for the relative permeability, the relative permeability of this phase is given by

$$\kappa_{ri} = (\bar{s}_i)^{q_i} \tag{6-113}$$

When the capillary diffusion option is selected for the capillary pressure model, it is assumed that the capillary effects are small, and all phase pressures are taken to be equal:

$$p_i = p_{i_c} \qquad \text{for} \quad i \neq i_c \tag{6-114}$$

However, it is still assumed that the capillary effects induce a (small) diffusive flux in the mass conservation equations for the different phases:

$$\frac{\partial}{\partial t}(\varepsilon_p \rho_i s_i) - \nabla \cdot \left(\rho_i \kappa_{ri} \frac{\kappa}{\mu_i} (\nabla p_{i_c} - \rho_i \mathbf{g}) + \rho_i D_{c_i} \nabla s_i \right) = Q_i \qquad \text{for} \quad i \neq i_c \tag{6-115}$$

where D_{c_i} denotes the capillary diffusion coefficient for phase *i*. The volumetric flux for the phases not computed from the volume constraint is in this case given by

$$\mathbf{u}_i = -\frac{\kappa_{ri}}{\mu_i} \kappa (\nabla p_i - \rho_i \mathbf{g}) - D_{c_i} \nabla s_i \tag{6-116}$$

Furthermore it is assumed that the capillary effects do not influence the equation for conservation of the total mass, so that this equations becomes

$$\frac{\partial}{\partial t}\left(\varepsilon_p \sum_{i=1}^{N} \rho_i s_i \right) - \nabla \cdot \left(\sum_{i=1}^{N} \rho_i \kappa_{ri} \frac{\kappa}{\mu_i} (\nabla p_{i_c} - \rho_i \mathbf{g}) \right) = \sum_{i=1}^{N} Q_i \tag{6-117}$$

Defining the volumetric flux of the phase computed from the volume constraint as follows

$$\mathbf{u}_{i_c} = -\frac{\kappa_{ri_c}}{\mu_{i_c}} \kappa (\nabla p_{i_c} - \rho_{i_c} \mathbf{g}) + \frac{1}{\rho_{i_c}} \sum_{i=1,\, i \neq i_c}^{N} \rho_i D_{c_i} \nabla s_i \tag{6-118}$$

results again in the following usual form of the equation for the conservation of the total mass

$$\frac{\partial}{\partial t}\left(\varepsilon_p \sum_{i=1}^{N} \rho_i s_i \right) - \nabla \cdot \left(\sum_{i=1}^{N} \rho_i \mathbf{u}_i \right) = \sum_{i=1}^{N} Q_i \tag{6-119}$$

Porous Medium Discontinuity Boundary Condition

Over a boundary between a more permeable and a less permeable porous domain, the macroscopic saturation of the different phases is often discontinuous. The **Porous Medium Discontinuity** boundary condition implements the following condition on such an interior boundary:

$$p_{c_i}^{l}(s_i^{l}) = \begin{cases} p_{ec,i}^{l} & \text{if} \quad p_{c_i}^{h}(s_i^{h}) \le p_{ec,i}^{l} \\ p_{c_i}^{h}(s_i^{h}) & \text{if} \quad p_{c_i}^{h}(s_i^{h}) > p_{ec,i}^{l} \end{cases} \quad \text{for} \quad i \neq i_c \qquad (6\text{-}120)$$

where the superscript l is used to indicate the saturation and capillary pressure on the low permeable side of the boundary, and the superscript h indicates the high permeable side. The first case implements the condition that if the capillary pressure on the more permeable side is lower than the entry capillary pressure on the less permeable side, then the saturation of phase i on the less permeable side equals 0 (or the residual saturation), and the second case implements the condition that if the capillary pressure on the more permeable side is higher than the entry capillary pressure on the less permeable side, the phase i is present on both sides of the interface, and that in this case the capillary pressure is continuous over the interface.

The additional conditions are continuity of the fluxes for all phases and continuity of the pressure of the phase i_c computed from the volume constraint. Note that this last condition assumes that this phase is present on both sides of the porous medium discontinuity boundary. In addition, this boundary condition assumes that the phase i_c computed from the volume constraint is the wetting phase and it is necessary that the settings for the van Genuchten or Brooks and Corey capillary pressure model match this assumption.

When the automatic settings are used for the **Porous Medium Discontinuity** boundary condition and if in one or both of the adjacent domains none of the predefined capillary pressure models is selected (**van Genuchten** or **Brooks and Corey**), the entry capillary pressure in that domain is determined by substituting 0 for saturation of the phase which is not computed from the volume constraint into the user defined expression for the capillary pressure.

Also note that if in one or both of the adjacent domains the **Capillary diffusion** model is selected, the **Porous Medium Discontinuity** boundary condition is not applicable as the entry capillary pressure in this case is not known on both sides of the boundary.

Free-Porous Interface

Over a boundary between a free flow and a porous domain, the macroscopic saturation of the different phases is often discontinuous. The **Free-Porous Interface** boundary condition implements a number of different conditions on such an interior boundary.

In the case that the droplets or bubbles of a nonwetting phase that are present on the free-flow side of the free-porous interface are larger than the maximum pore size, continuity of the phase pressure implies that the saturation on the porous side is equal to the phase residual saturation:

$$s_i^{\mathrm{p}} = s_{ri} \tag{6-121}$$

where s_{ri} denotes the residual saturation of phase i (which is taken to be equal to zero when the capillary pressure model in the adjacent **Porous Medium** is user defined), and where s_i^{p} denotes the saturation of phase i on the porous side of the interface. This condition is implemented for the **Residual saturation** option.

In the case that one would like to set a maximum saturation on the porous side of the interface that is larger than the residual saturation, one can use the **Outflow, no flux below threshold saturation** option. This implements the following Signorini-type condition:

$$s_i^{\mathrm{p}} \le s_{0,i}, \qquad -\mathbf{n}\cdot(\rho_i\mathbf{u}_i) \le 0, \qquad (s_i^{\mathrm{p}} - s_{0,i})(\mathbf{n}\cdot(\rho_i\mathbf{u}_i)) = 0 \tag{6-122}$$

Here $s_{0,i}$ is the threshold saturation below which the saturation s_i^{p} should remain, and $\mathbf{n}\cdot(\rho_i\mathbf{u}_i)$ the mass flux out of the porous domain of phase i (it is assumed that the vector $\mathbf{n}$ normal to the interface is pointing out of the porous domain). This means that the second inequality implies that phase i is only allowed to flow out of the porous domain. The last equality ensures that when the saturation s_i^{p} is below, and not equal to, the threshold value, the flux of phase i across the free-porous interface is zero.

When the droplets, bubbles or particles of a phase i are smaller than the maximum pore size but still larger than the minimum pore size, only a fraction of all pores are accessible for these droplets, bubbles or particles. In that case one can use the **Ratio of free flow volume fraction** option to apply the following condition on the free-porous interface:

$$s_i^{\mathrm{p}} = r_{0,i}\, s_i^{\mathrm{f}} \tag{6-123}$$

Here $r_{0,i}$ is the ratio between the phase saturation s_i^{p} on the porous side and the phase volume fraction s_i^{f} on the free-flow side of the free-porous interface.

For all three options, the additional condition is continuity of the fluxes for all phases and it is assumed that the pressure of the phase i_c computed from the volume constraint is continuous over the free-porous interface. Note that this last condition assumes that this phase is present on both sides of the interface. In addition, this boundary condition assumes that the phase i_c computed from the volume constraint is the wetting phase and it is necessary that the settings for the van Genuchten or Brooks and Corey capillary pressure model in the adjacent porous domains match this assumption.

References for the Phase Transport Interfaces

1. M.Th. van Genuchten, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," *Soil Sci. Soc. Am. J.*, vol. 44, 1980.

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Theory for the Phase Transport Mixture Model Interfaces

The model equations that are solved in the **Phase Transport Mixture Model** interfaces are based on the mass conservation of each phase and on conservation of momentum. The mass conservation equation for each (immiscible) phase $i = 1, \ldots, N$ is given by

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) = Q_i \tag{6-124}$$

where ρ_i denotes the density (SI unit: kg/m^3), s_i denotes the volume fraction (dimensionless), and $\mathbf{u}_i$ denotes the velocity vector (SI unit: m/s) of phase i. In addition, the term Q_i denotes a mass source for phase i (SI unit: kg/(m^3·s)). It is assumed that the sum of the volume fractions of the phases equals 1:

$$\sum_{i=1}^{N} s_i = 1 \tag{6-125}$$

This means that $N - 1$ phase volume fractions are independent and are possible to solve for using Equation 6-124. The volume constraint Equation 6-125 is used to reduce the number of dependent variables: one volume fraction, let us say of phase i_c (to be specified in the main node of the coupled **Phase Transport** interface), is expressed using the other volume fractions:

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i \right) \tag{6-126}$$

In the **Mixture Model** multiphysics coupling feature, it is assumed that the phase i_c is the continuous phase.

Furthermore, the mass averaged mixture velocity $\mathbf{u}_\mathrm{m}$ is defined as:

$$\mathbf{u}_\mathrm{m} = \frac{1}{\rho} \sum_{i=1}^{N} s_i \rho_i \mathbf{u}_i \tag{6-127}$$

Here ρ is the mixture density (SI unit: kg/m^3) given by:

$$\rho = \sum_{i=1}^{N} s_i \rho_i \tag{6-128}$$

Summing the mass conservation equations for all phases gives the following continuity equation for the mixture

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{u}_{\mathrm{m}}) = \sum_{i=1}^{N} Q_i \tag{6-129}$$

The velocity $\mathbf{u}_i$ of phase i is defined as:

$$\mathbf{u}_i = \mathbf{u}_{\mathrm{m}} + \mathbf{u}_{\mathrm{slip},i} - \frac{1}{\rho} \sum_{j=1, j \neq i_c}^{N} \rho_j s_j \mathbf{u}_{\mathrm{slip},j} - \frac{D_{md}}{s_i} \nabla s_i \quad \text{for} \quad i \neq i_c \tag{6-130}$$

where the slip velocity $\mathbf{u}_{\mathrm{slip},i}$ (SI unit: m/s) is given by one of the slip velocity models discussed below, and where the last term accounts for the turbulent effects, with $D_{m\mathrm{d}}$ (SI unit: m^2/s) a turbulent dispersion coefficient given by

$$D_{m\mathrm{d}} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is the turbulent particle Schmidt number (dimensionless). The particle Schmidt number is usually suggested a value ranging from 0.35 to 0.7.

Using the expression above for the velocity $\mathbf{u}_i$ of phase i, the conservation equation for the dispersed phases can be written as

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i (\mathbf{u}_{\mathrm{m}} - \mathbf{u}_{\mathrm{r}} + \mathbf{u}_{\mathrm{slip},i}) - \rho_i D_{m\mathrm{d}} \nabla s_i) = Q_i \tag{6-131}$$

Here the velocity field $\mathbf{u}_{\mathrm{r}}$ is the mass average of all slip velocities:

$$\mathbf{u}_{\mathrm{r}} = \frac{1}{\rho} \sum_{i=1, i \neq i_c}^{N} \rho_i s_i \mathbf{u}_{\mathrm{slip},i} \tag{6-132}$$

With the previous definitions, the velocity of the continuous phase $\mathbf{u}_{i_c}$ can be written in terms of the mixture velocity $\mathbf{u}_{\mathrm{m}}$ and the slip velocities $\mathbf{u}_{\mathrm{slip},i}$ as follows:

$$\mathbf{u}_{i_c} = \mathbf{u}_\mathrm{m} - \mathbf{u}_\mathrm{r} + \frac{1}{\rho_{i_c} s_{i_c}} \sum_{i=1,\, i \neq i_c}^{N} \rho_i D_{md} \nabla s_i \tag{6-133}$$

The momentum equation for the mixture is

$$\begin{aligned} \rho \mathbf{u}_{\mathrm{m}t} + \rho(\mathbf{u}_\mathrm{m} \cdot \nabla)\mathbf{u}_\mathrm{m} + \nabla \cdot \left(\sum_{i=1,\, i \neq i_c}^{N} \rho_i s_i \mathbf{u}_{\mathrm{slip},i} \mathbf{u}_{\mathrm{slip},i}^T - \rho \mathbf{u}_\mathrm{r} \mathbf{u}_\mathrm{r}^T \right) \\ = -\nabla p + \nabla \cdot \tau_\mathrm{Gm} + \rho \mathbf{g} + \mathbf{F} \end{aligned} \tag{6-134}$$

Here τ_Gm is the sum of the viscous and turbulent stresses (SI unit: kg/(m·s^2)). The last term between parenthesis on the first line of Equation 6-134 is called the diffusion stress.

When the **Low dispersed phase concentration** checkbox is selected (see The Phase Transport Mixture Model Interfaces), the momentum equation, Equation 6-134, and continuity equation, Equation 6-129, are replaced by

$$\begin{aligned} \rho_{i_c} \mathbf{u}_{\mathrm{m}t} + \rho_{i_c}(\mathbf{u}_\mathrm{m} \cdot \nabla)\mathbf{u}_\mathrm{m} + \nabla \cdot \left(\sum_{i=1,\, i \neq i_c}^{N} \rho_i s_i \mathbf{u}_{\mathrm{slip},i} \mathbf{u}_{\mathrm{slip},i}^T - \rho_{i_c} \mathbf{u}_\mathrm{r} \mathbf{u}_\mathrm{r}^T \right) \\ = -\nabla p + \nabla \cdot \tau_\mathrm{Gm} + \rho \mathbf{g} + \mathbf{F} \end{aligned} \tag{6-135}$$

and

$$\frac{\partial}{\partial t} \rho_{i_c} + \nabla \cdot (\rho_{i_c} \mathbf{u}_\mathrm{m}) = \sum_{i=1}^{N} Q_i \tag{6-136}$$

When the **Include bubble-induced turbulence** checkbox is selected, a source term S_k, which accounts for extra production of turbulence due to relative motion between the gas bubbles and the liquid, is added to the transport equation for the turbulent kinetic energy, k. This term is given by

$$S_\mathrm{k} = -C_\mathrm{k} \sum_{i=1,\, i \neq i_c}^{N} s_i \nabla p \cdot \mathbf{u}_{\mathrm{slip},i}$$

In addition, the transport equation for the turbulent energy's dissipation rate, ε, includes the following source term:

$$C_\varepsilon S_k \frac{\varepsilon}{k}$$

When, on the other hand, the coupled turbulence model includes the specific dissipation rate, ω, the following source term is added to the transport equation for ω:

$$\alpha_\omega S_k \frac{\omega}{k}$$

Suitable values for the model parameters C_k, C_ε, and α_ω are not as well established as the parameters for single-phase flow. In the literature, values within the ranges $0.01 < C_k < 1$, $1 < C_\varepsilon < 1.92$ have been suggested (see also Theory for the Bubbly Flow Interfaces), and α_ω can be defined as $\alpha_\omega = C_\varepsilon - 1$.

When the **Include shear-induced migration** checkbox is selected, the conservation equation for the dispersed phases are augmented with shear induced flux density terms as follows:

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) = \nabla \cdot \left(\rho_i \left(\mathbf{j}_{di} + \frac{s_i}{\rho} \sum_{j=1, j \neq i_c}^{N} (\rho_{i_c} - \rho_j) \mathbf{j}_{dj} \right) \right) + Q_i \quad (6\text{-}137)$$

where

$$\mathbf{j}_{di} = K_c s_i \dot{\gamma} \sum_{j=1, j \neq i_c}^{N} A_{ij} s_i \nabla \ln(s_i \dot{\gamma} \mu^\lambda) \quad (6\text{-}138)$$

where $\dot{\gamma}$ is the shear rate given by

$$\dot{\gamma} = \sqrt{2\mathbf{S}:\mathbf{S}} \quad \text{with} \quad \mathbf{S} = \frac{1}{2}(\nabla \mathbf{u}_m + (\nabla \mathbf{u}_m)^T) \quad (6\text{-}139)$$

and where

$$A_{ij} = \frac{(d_i/2 + d_j/2)^2}{16} \frac{(1 + d_i/d_j)^3}{1 + (d_i/d_j)^3} \quad (6\text{-}140)$$

Here, K_c and λ are dimensionless model parameters with default values 0.4 and 1.59, respectively (Ref. 4).

Mixture Viscosity Models

The Newtonian viscosities of interpenetrating media are not readily available. Instead empirical and analytical models for the dynamic viscosity mixture have been developed, usually as a function of the dispersed volume fraction.

A simple mixture viscosity model, which is only available when there is one dispersed phase covering the entire range of particle volume fractions s_d is the Krieger type model (Ref. 1):

$$\mu = \mu_c\left(1 - \frac{s_d}{\phi_{d,max}}\right)^{-2.5\phi_{d,max}} \tag{6-141}$$

Here $\phi_{d,max}$ is the maximum packing limit, by default 0.62. An extension of Equation 6-62 can be applied for liquid droplets/bubbles:

$$\mu = \mu_c\left(1 - \frac{s_d}{\phi_{d,max}}\right)^{-2.5\phi_{d,max}\frac{\mu_d + 0.4\mu_c}{\mu_d + \mu_c}} \tag{6-142}$$

where μ_c and μ_d are the viscosities of the continuous and dispersed phase, respectively.

When there is more than one dispersed phase, the following Krieger type mixture viscosity model (Ref. 3) is used:

$$\mu = \mu_c e^{-2.5\eta} \tag{6-143}$$

where

$$\eta = \sum_{i=1,\, i\neq i_c}^{N} \frac{s_i}{S_i(\phi_{d,max}) - S_i(2)} \ln\left(\frac{1 - (s - S_i(2))}{1 - (s - S_i(\phi_{d,max}))}\right)$$

$$S_i(x) = \sum_{j=1,\, j\neq i_c}^{N} \frac{s_j\left(\frac{2{,}5}{x}\frac{d_i}{d_j} - \left(\frac{d_i}{d_j}\right)^{2{,}5}\right)}{\left(\frac{1{,}5}{1 - \phi_{d,max}} + \left(\frac{d_i}{d_j}\right)^{2{,}5}\right)}$$

with d_i the particle diameter of phase i, and

$$s = \sum_{i=1, i \neq i_c}^{N} s_i \tag{6-144}$$

For fluid-fluid systems, the volume averaged viscosity defined by

$$\mu = \sum_{i=1}^{N} s_i \mu_i \tag{6-145}$$

is also available.

Slip Velocity Models

The **Mixture Model** multiphysics coupling contains three predefined models for the slip velocity between a dispersed phase and the continuous phase $\mathbf{u}_{\text{slip},i}$:

- The *Schiller–Naumann model*
- The *Haider–Levenspiel model*
- The *Hadamard–Rybczynski model*

All three models use the following relation for the slip velocity:

$$\frac{3}{4}\frac{C_{\text{d},i}}{d_i}\left|\mathbf{u}_{\text{slip},i}\right|\mathbf{u}_{\text{slip},i} = -\frac{(\rho - \rho_i)}{\rho_{i_c}}\left(-\mathbf{u}_{\text{m}t} - (\mathbf{u}_{\text{m}} \cdot \nabla)\mathbf{u}_{\text{m}} + \mathbf{g} + \frac{\mathbf{F}}{\rho}\right) \tag{6-146}$$

where $C_{\text{d},i}$ (dimensionless) is the particle drag coefficient and d_i is the particle diameter of phase i.

The Schiller–Naumann model models the drag coefficient according to

$$C_{\text{d},i} = \begin{cases} \dfrac{24}{\text{Re}_{\text{p},i}}(1 + 0{,}15\text{Re}_{\text{p},i}^{0{,}687}) & \text{Re}_{\text{p},i} < 1000 \\ 0{,}44 & \text{Re}_{\text{p},i} > 1000 \end{cases}$$

where $\text{Re}_{\text{p},i}$ is the particle Reynolds number

$$\text{Re}_{\text{p},i} = \frac{d_i \rho_{i_c} \left|\mathbf{u}_{\text{slip},i}\right|}{\mu}$$

Note that this definition of the particle Reynolds number uses the viscosity of the mixture and not the viscosity of the continuous phase, as would be customary for a

single particle in a pure fluid with viscosity μ_c. This choice incorporates the hindrance effect of the other particles on the slip velocity, see Ref. 2.

Because the particle Reynolds number depends on the slip velocity, an implicit equation must be solved to obtain the slip velocity. Therefore, the **Mixture Model** multiphysics coupling feature adds an additional equation for

$$|\mathbf{u}_{\text{slip},i}|^2$$

when the Schiller–Naumann slip model is used. The Schiller–Naumann model is particularly well suited for solid particles in a liquid.

The Haider–Levenspiel model is applicable to nonspherical particles. It models the drag coefficient according to

$$C_{\text{d},i} = \frac{24}{\text{Re}_{\text{p},i}}(1 + A(S_i)\text{Re}_{\text{p},i}^{B(S_i)}) + \frac{C(S_i)}{1 + D(S_i)/\text{Re}_{\text{p},i}}$$

where A, B, C, and D are empirical correlations of the particle sphericity S_i. The sphericity is defined as the ratio of the surface area of a volume equivalent sphere to the surface area of the considered nonspherical particle

$$0 < S_i = \frac{A_{\text{sphere}}}{A_{\text{particle}}} \leq 1$$

The correlation coefficients are given by

$$A(S_i) = e^{2.3288 - 6.4581S_i + 2.4486S_i^2}$$
$$B(S_i) = 0.0964 + 0.5565S_i$$
$$C(S_i) = e^{4.905 - 13.8944S_i + 18.4222S_i^2 - 10.2599S_i^3}$$
$$D(S_i) = e^{1.4681 + 12.2584S_i - 20.7322S_i^2 + 15.8855S_i^3}$$

The diameter used in the particle Reynolds number is that of the volume equivalent sphere. The equation for the squared slip velocity is also added when the Haider–Levenspiel slip model is used.

The Hadamard–Rybczynski drag law is valid for particle Reynolds numbers less than 1, for particles, bubbles, and droplets. The drag coefficient for liquid droplets or bubbles is

$$C_{\mathrm{d},i} = \frac{24}{\mathrm{Re}_{\mathrm{p},i}}\left(\frac{1+\frac{2}{3}\frac{\mu_{i_c}}{\mu_i}}{1+\frac{\mu_{i_c}}{\mu_i}}\right)$$

which yields the following explicit expression for the slip velocity

$$\mathbf{u}_{\mathrm{slip},i} = -\frac{(\rho-\rho_i)d_i^2}{18\mu}\left(\frac{1+\frac{\mu_{i_c}}{\mu_i}}{1+\frac{2}{3}\frac{\mu_{i_c}}{\mu_i}}\right)\left(-\mathbf{u}_{\mathrm{m}t}-(\mathbf{u}_{\mathrm{m}}\cdot\nabla)\mathbf{u}_{\mathrm{m}}+\mathbf{g}+\frac{\mathbf{F}}{\rho}\right)$$

For solid particles, the slip velocity is given by

$$\mathbf{u}_{\mathrm{slip},i} = -\frac{(\rho-\rho_i)d_i^2}{18\mu}\left(-\mathbf{u}_{\mathrm{m}t}-(\mathbf{u}_{\mathrm{m}}\cdot\nabla)\mathbf{u}_{\mathrm{m}}+\mathbf{g}+\frac{\mathbf{F}}{\rho}\right)$$

when $\mathrm{Re}_{\mathrm{p},i} < 1$. For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

Coupled Interfaces: Equations and Coupled Quantities

The equations for the volume fractions of the dispersed phases (Equation 6-124) are solved in the **Phase Transport** interface. The momentum equation and the continuity equation for the mixture velocity and pressure (Equation 6-129 and Equation 6-134) are solved in the coupled laminar or turbulent single-phase flow interface. The **Mixture Model** multiphysics coupling feature supplies the mixture density ρ and viscosity μ to the single-phase flow interface, and the convective dispersed phase velocities $\mathbf{u}_{i_c}+\mathbf{u}_{\mathrm{slip},i}$ to the **Phase Transport** interface. In addition it adds the diffusion stress term to the momentum equation (see Equation 6-134, when the **Include diffusion stress in momentum equation** checkbox is selected), and the diffusive term to the transport equations for the dispersed phases (see Equation 6-124). In case there are mass sources in the **Phase Transport** interface, the **Mixture Model** multiphysics feature adds the right-hand side to the mixture continuity equation (Equation 6-129).

References

1. H. Enwald, E. Peirano, and A.-E. Almstedt, "Eulerian Two-Phase Flow Theory Applied to Fluidization", *Int. J. Multiphase Flow*, vol. 22, pp. 21–66, 1996.

2. M. Ungarish, *Hydrodynamics of suspensions*, Springer-Verlag, 1993.

3. R. S. Farr, "Simple heuristic for the viscosity of polydisperse hard spheres", *J. Chem. Phys.*, vol. 141, 214503, 2014.

4. Ph. Kanehl and H. Stark, "Hydrodynamic segregation in a bidisperse colloidal suspension in microchannel flow: A theoretical study", *J. Chem. Phys.*, vol. 142, 214901, 2015.

Theory for the Nonisothermal Mixture Model Interfaces

The model equations that are solved in the **Nonisothermal Mixture Model** interfaces are a combination of the **Phase Transport Mixture Model** interfaces and **Nonisothermal Flow**. The equations solved are the mass conservation of each phase, conservation of momentum of the mixture, and the temperature equation. For more information, see Theory for the Phase Transport Interfaces and Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces.

Mixture Material Properties for Heat Transfer

The Nonisothermal Mixture Model multiphysics coupling provides the thermal conductivity k, heat capacity at constant pressure C_p, and ratio of specific heats γ of the mixture to the heat transfer interface.

The thermal conductivity of the mixture k is volume averaged over all the phases:

$$k = \sum_{i=1}^{N} s_i k_i$$

The heat capacity at constant pressure C_p of the mixture is obtained from mass-averaging:

$$C_p = \frac{\sum_{i=1}^{N} s_i \rho_i C_{p,i}}{\rho}$$

The ratio of specific heats γ is obtained as the ratio of C_p respect to C_v:

$$\gamma = \frac{C_p}{C_v} = \frac{\sum_{i=1}^{N} s_i \rho_i C_{p,i}}{\sum_{i=1}^{N} s_i \rho_i \frac{C_{p,i}}{\gamma_i}}$$

Note that C_v is obtained from a mass-averaging across the phases.

7

Porous Media and Subsurface Flow Interfaces

This chapter discusses physics interfaces under the **Fluid Flow** > **Porous Media and Subsurface Flow** branch ( ). The section Modeling Porous Media and Subsurface Flow helps you choose the best physics interface to start with.

In this chapter:

- Modeling Porous Media and Subsurface Flow
- The Darcy's Law Interface
- The Brinkman Equations Interface
- The Free and Porous Media Flow, Brinkman Interface
- The Free and Porous Media Flow, Darcy Interface
- The Two-Phase Darcy's Law Interface
- The Multiphase Flow in Porous Media Interface
- The Multiphase Free and Porous Media Flow Interface
- The Thin-Film and Porous Media Flow Interface
- Theory for the Darcy's Law Interface
- Theory for the Brinkman Equations Interface
- Theory for the Free and Porous Media Flow, Brinkman Interface

- Theory for the Free and Porous Media Flow, Darcy Interface
- Theory for the Two-Phase Darcy's Law Interface
- Theory for the Multiphase Flow in Porous Media Interface
- Theory for the Thin-Film and Porous Media Flow Interface

Modeling Porous Media and Subsurface Flow

In this section:

- Selecting the Right Physics Interface
- The Porous Media Flow Interface Options
- Coupling to Other Physics Interfaces

Selecting the Right Physics Interface

The **Porous Media and Subsurface Flow** branch ( ) included with the CFD Module has a number of subbranches to describe momentum transport. These can be added either singularly or in combination with other physics interfaces modeling mass and energy transfer, and even chemical reactions.

Different types of flow require different equations to describe them. If the flow type to model is known, then select it directly. However, when you are not certain of the flow type, or when it is difficult to obtain a solution, you can instead start with a simplified model and add complexity as you build the model. Then you can successively advance forward, comparing models and results. For porous media flow, the **Darcy's Law** interface is a good place to start if this is the case.

In other cases, you might know exactly how a fluid behaves and which equations, models, or physics interfaces best describe it, but because the model is so complex it is difficult to reach convergence. Simplifying assumptions can be made to solve the problem, and other physics interfaces can be better at fine-tuning the solution process for the more complex problem. The next section gives you an overview of each of the physics interfaces to help you choose.

TABLE 7-1: THE POROUS MEDIA FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM	PORE SIZE
Darcy's Law	dl	Compressible flow	n/a	Low porosity and low permeability, slow flow
Two-Phase Darcy's law	tpdl	n/a	n/a	Low porosity and low permeability, slow flow

TABLE 7-1: THE POROUS MEDIA FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM	PORE SIZE
Brinkman Equations	br	Incompressible flow	Yes - Stokes–Brinkman	High permeability and porosity, faster flow
Free and Porous Media Flow, Brinkman	fp	Incompressible flow	Not selected	High permeability and porosity, fast flow

Figure 7-1 is an example of the **Settings** window for **Brinkman Equations** where you can select either Compressible or Incompressible flow, and either normal or Stokes Brinkman flow. For **Darcy's Law** interface, you can select Incompressible, Compressible, Compressible, linearized, or Ideal gas as a fluid type under Porous Medium/Fluid node.

The Porous Media Flow Interface Options

DARCY'S LAW

The Darcy's Law Interface ( ) is used for modeling fluid movement through interstices in a porous medium by homogenizing the porous and fluid media into a single medium. Together with the continuity equation and equation of state for the pore fluid (or gas) this physics interface can be used to model low velocity flows, for which the pressure gradient is the major driving force. The penetration of reacting gases into a tight catalytic layer, such as a washcoat or membrane, is a classic example for the use of Darcy's Law.

Darcy's law can be used in porous media where the fluid is mostly influenced by the frictional resistance within the pores. It applies to very slow flows, or media where the pore size is very small.

BRINKMAN EQUATIONS

Where the size of the interstices are larger, and the fluid is also influenced by internal shear or shear stresses on boundaries, the viscous shear within the fluid must be considered. This is done in the Brinkman Equations interface. Fluid penetration of filters and packed beds are applications for this mode. The Brinkman Equations Interface ( ) is used to model incompressible flow. You can also choose to model compressible flow at speeds less than Mach 0.3, but you have to maintain control over the density and any of the mass balances that are deployed to accomplish this. Furthermore, you can select the Stokes–Brinkman flow feature to reduce the influence of inertial effects (see Figure 7-1).

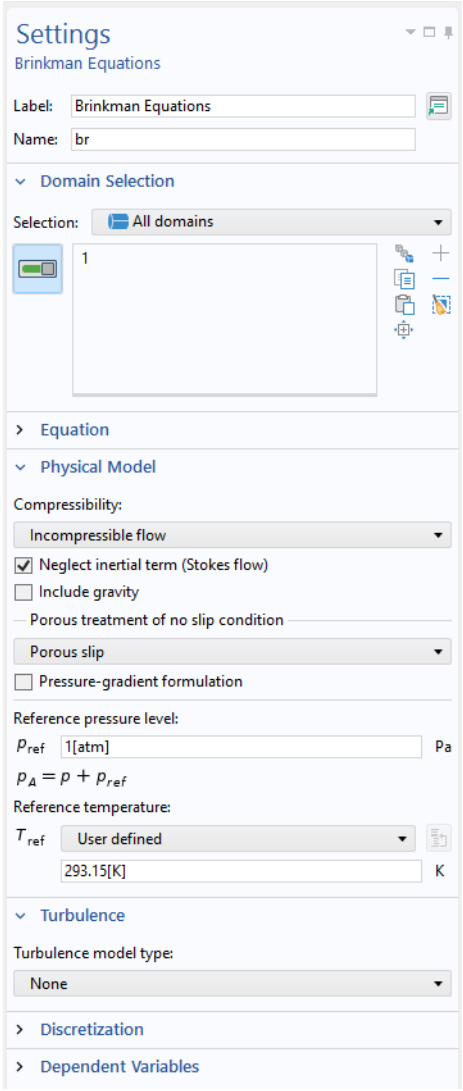

Figure 7-1: The Settings window for the Brinkman Equations interface. You can model compressible or incompressible flow as well as Stokes–Brinkman flow. Combinations are also possible.

The *Brinkman equations* extend Darcy's law to describe the dissipation of momentum by viscous shear, similar to the Navier–Stokes equation. Consequently,

they are well suited to model transitions between slow flow in porous media, governed by Darcy's law, and fast flow in channels described by the Navier–Stokes equations.

The Brinkman Equations interface also includes the possibility to add a Forchheimer drag term, which is a viscous drag on the porous matrix proportional to the square of the flow velocity. This term accounts for an inertial turbulent drag effect that comes into play for fast flows through large pores. Adding the Forchheimer term takes into account all drag contributions that the Ergun equation covers.

FREE AND POROUS MEDIA FLOW, BRINKMAN

The Free and Porous Media Flow, Brinkman Interface ( ) is useful for modeling equipment that contains domains with both free flow and porous media flow, such as packed-bed reactors and catalytic converters. It should be noted that if the porous medium is large in comparison with the free channel, and you are not primarily interested in results in the vicinity of the interface, you can always couple a Fluid Flow interface to a Darcy's Law interface, to make your overall model computationally cheaper.

The Free and Porous Media Flow, Brinkman interface is used on at least two different domains; a free channel and a porous medium. The physics interface adds functionality that allows the equations to be optimized according to the definitions of the material properties of the relevant domain. For example, you can select the Stokes–Brinkman flow feature to reduce the dependence on inertial effects in the porous domain, or just the Stoke's flow feature to reduce the dependence on inertial effects in the free channel.

Compressible flow is also possible to model in this physics interface at speeds less than Mach 0.3, but you have to maintain control over the density and any of the mass balances that are deployed to accomplish this. You can also choose to model incompressible flow, and simplify the equations to be solved.

As always, the physics interface gives you provides you with options to define, either by constants or expressions, the material properties that describe the porous media flow. This includes the density, dynamic viscosity, permeability, porosity, and matrix properties.

FREE AND POROUS MEDIA FLOW, DARCY

The Free and Porous Media Flow, Darcy Interface ( ) is a multiphysics interface that is used to model coupled free and porous media flow. It uses a Darcy's Law interface in the porous domain and a Laminar Flow interface in the free-flow domain, which are coupled over the free-porous interface by the Free and Porous Media Flow Coupling

multiphysics boundary feature. This coupling feature provides several options for modeling the tangential velocity component of the free flow at the free-porous interface.

As the interface uses Darcy's law, it does not take into account inertial effects in the porous domain. In addition, it is assumed that the flow in the free-flow domain is laminar, and as such the interface is suited for situations when the flow in both the porous and the free-flow regions is reasonably slow.

This interface supports laminar, compressible flow at speeds less than Mach 0.3, as well as incompressible flow.

TWO-PHASE DARCY'S LAW

The Two-Phase Darcy's Law Interface ( ) has the equations and boundary conditions for modeling two-phase fluid movement through interstices in a porous medium using Darcy's law. The two fluids are considered immiscible, and in general, have different densities and viscosities.

As for the single phase Darcy's Law, the total velocity field is determined by the total pressure gradient and the structure of the porous medium, but the average viscosity and average density are calculated from the saturation of each immiscible phase and their fluid properties. An extra equation is computed — the fluid content of one phase — in order to calculate the saturation transport.

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple fluid flow in porous or subsurface media to another type of phenomenon described in another physics interface. This can include chemical reactions and mass transport, as described in Chemical Species Transport Interfaces, or energy transport in porous media described in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of modeling chemical reactions and mass transport are found in the Chemical Reaction Engineering Module. Furthermore, some applications that involve electrochemical reactions and porous electrodes, particularly in electrochemical power source applications, are supported in the Battery Design Module.

Fluid flow is an important phenomenon for cooling in electromagnetic applications, such as heat created through induction and microwave heating, which are simulated in the AC/DC Module and RF Module, respectively. Other applications can involve the

effect of fluid-imposed momentum on structural applications; poroelasticity. The Structural Mechanics Module and Subsurface Flow Module have interfaces specifically for these multiphysics applications.

The following sections list all the physics interfaces and the features associated with them under the Porous Media Subsurface Flow branch. The descriptions follow a structured order as defined by the order in the branch. Because many of the physics interfaces are integrated with each other, some features described also cross reference to other physics interfaces. At the end of this section is a summary of the theory for the physics interfaces under the Porous Media Subsurface Flow branch.

The Darcy's Law Interface

The **Darcy's Law (dl)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. Set up multiple **Darcy's Law** interfaces to model multiphase flows involving more than one mobile phase. The Darcy's Law interface can be used for stationary and time-dependent analyses.

The main feature is the **Porous Medium** Properties node, which provides interfaces for defining the fluid material and the porous matrix properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Porous Medium**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Darcy's Law** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `dl`.

PHYSICAL MODEL

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

GRAVITY EFFECTS

By default there are no gravity effects added to Darcy's Law interface. Select the checkbox **Include gravity** to activate the acceleration of gravity. When this checkbox is selected, a global **Gravity** feature node is shown in the interface model tree.

Enter a value for the acceleration of gravity. The default value `g_const` is the predefined standard acceleration of gravity on earth.

For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

DISCRETIZATION

To display all settings available in this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

You can choose the order of the shape functions used for the pressure variable solved by the Darcy's Law interface. The default shape functions are **Quadratic** Lagrange.

The **Compute boundary fluxes** checkbox is not activated by default. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the checkbox is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

Also, the **Apply smoothing to boundary fluxes** checkbox is available if the previous checkbox is checked. The smoothing can provide a better behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the *COMSOL Multiphysics Reference Manual*.

The **Value type when using splitting of complex variables** setting should in most pure mass transport problems be set to **Real** which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure**. The name can be changed but the names of fields and dependent variables must be unique within a model.

- Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface
- Theory for the Darcy's Law Interface
- Physical Constants in the *COMSOL Multiphysics Reference Manual*

- *Species Transport in the Gas Diffusion Layers of a PEM*: Application Library path **Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pem_gdl_species_transport_2d**
- *Steam Reformer*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/steam_reformer**
- *Terzaghi Compaction*: Application Library path **Subsurface_Flow_Module/Poromechanics/terzaghi_compaction**

Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface

The Darcy's Law Interface has the following domain, boundary, edge, point, and pair nodes, these nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

DOMAIN

- Porous Medium
- Unsaturated Porous Medium
- Dual Porosity Medium
- Dual Permeability Medium
- Unsaturated Dual Permeability Medium
- Mass Source
- Cross Section
- Initial Values
- Unsaturated Porous Medium
- ThicknessContributing Velocity
- Porous Electrode Coupling

BOUNDARY, EDGE, AND POINT

The following nodes (listed in alphabetical order) are available on exterior boundaries:

- Atmosphere/Gauge
- Electrode Surface Coupling
- Flux Discontinuity
- Fracture
- Hydraulic Head
- Inlet
- Interior Wall
- Line Mass Source
- Mass Flux
- No Flow
- Outlet
- Pervious Layer
- Point Mass Source
- Precipitation
- Pressure
- Pressure Head
- [1]
- Symmetry
- Thin Barrier

[1] This node is described for the Transport of Diluted Species Interface

The relevant physics interface condition at interior boundaries is continuity:

$$\mathbf{n} \cdot (\rho_1 \mathbf{u}_1 - \rho_2 \mathbf{u}_2) = 0$$

The continuity boundary condition ensures that the pressure and mass flux are continuous. In addition, the Pressure boundary condition is available on interior boundaries.

The continuity boundary condition provides continuity for the pressure and mass flux. In addition, the following boundary conditions are available on interior boundaries:

- Pressure
- Pressure Head
- Hydraulic Head
- Interior Wall
- Pervious Layer
- Flux Discontinuity
- Fracture
- Thin Barrier

Note that some of the above-mentioned domain or boundary conditions are only available with some products. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Porous Medium

The **Porous Medium** node adds the equations for modeling flow through porous domains. By default these are Equation 7-1 and Equation 7-2 (excluding any mass sources).

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{7-1}$$

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{7-2}$$

For a steady-state problem the first term in Equation 7-1 disappears. When Mass Source is active Equation 7-2 is of the following form:

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p - \rho \mathbf{g}) \tag{7-3}$$

The **Porous Medium** feature has two default subfeatures — the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Porous Matrix subnode) should be set according to the coordinate system selected in this section.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship using Equation 7-1 and Equation 7-2.
- **Non-Darcian flow** defines a nonlinear relationship using Equation 7-1 and

$$\nabla p = -\frac{\mu}{\kappa}\mathbf{u} - \beta\rho|\mathbf{u}|\mathbf{u}$$

  where the nonlinear parameter β (SI unit: $1/m$) is further specified in the Porous Matrix subfeature.

STORAGE MODEL

Define the time dependent storage term by selecting one of the following options from the list:

- **From density and porosity** (default), uses the formulation of Equation 7-1

- **Linearized storage**, where the following linear equation is used to define the storage:

$$S_p = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p$$

- **Poroelastic storage**, where $S_p = \varepsilon_p \chi_f$
- **Quasistatic**, where the storage term is set to zero
- **User defined** to directly specify the storage coefficient S_p

	• Porous Material in the *COMSOL Multiphysics Reference Manual* • About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide* • Storage Models in the *Subsurface Flow Module User's Guide*

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Porous Medium**
Richards' Equation > **Porous Medium**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Porous Medium**

Fluid

This node defines the material properties of the fluid of the Porous Medium, the Unsaturated Porous Medium, the Dual Porosity Medium, the Dual Permeability Medium, or the Unsaturated Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

The available options for the **Fluid type** are **Incompressible**, **Compressible**, **Compressible, linearized**, or **Ideal gas**. The selection determines how the density and compressibility of the fluid are set.

Incompressible

The default **Reference density** ρ_{ref} uses values **From material**. For **User defined** enter another value or expression.

Compressible

The default **Density** ρ uses values **From material**. For **User defined** enter another value or expression as a function of the absolute pressure. The compressibility of the fluid is computed from it.

Compressible, Linearized

The default **Reference density** ρ_{ref} and the **Fluid compressibility** χ_{f} use values **From material**. For **User defined** enter another value or expression. The fluid density increases linearly as a function of the fluid pressure.

Ideal Gas

For **Ideal gas** it uses the ideal gas law to describe the gas density. In this case, specify the thermodynamics properties. Select a **Gas constant type** — **Specific gas constant** R_s (the default) or **Mean molar mass** M_n (SI unit: J/(mol·K)). For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K) is used as the built-in physical constant. For both properties, the defaults use values **From material**. For **User defined** enter another value or expression.

Dynamic Viscosity

For all fluid types specify the **Dynamic viscosity** μ (SI unit: Pa·s) uses values **From material**. For **User defined** enter another value or expression.

Constitutive Relation

The Polymer Flow Module allows the use of inelastic non-Newtonian models. For Darcian Flow, you can choose between two options: **Specify dynamic viscosity** (default) or **Inelastic non-Newtonian**. Use the default option to either get the dynamic viscosity from a material, or to add a user defined expression. The default option lets you either use the dynamic viscosity from a material or define it with a custom expression. The **Inelastic non-Newtonian** option provides several models and defines the **Apparent shear rate**.

Inelastic Non-Newtonian

The following inelastic non-Newtonian Models are available for the **Fluid** feature under the **Porous Medium** feature:

- Power Law
- Carreau
- Carreau-Yasuda
- Cross
- Cross-Williamson
- Sisko

The setup of these models in porous media is similar to their definition under the Fluid Properties feature.

Apparent Shear Rate

To define the apparent shear rate $\dot{\gamma}_{app}$, either enter a user-defined expression for the correction factor (α) or choose the **Capillary bundle approach** from the list and provide a value for the Tortuosity factor (C).

- Read more about the theory of Non-Newtonian Fluids in Porous Media in the *Polymer Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Fluid** node is automatically added to the Porous Medium, the Unsaturated Porous Medium, the Dual Porosity Medium, the Dual Permeability Medium, and the Unsaturated Dual Permeability Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Fluid**
Richards' Equation > *porous medium feature* > **Fluid**

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium or Unsaturated Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The default **Porosity** ε_p of the solid matrix is taken **From material**. In a **Porous Material** node, the porosity is defined as follows:

$$\varepsilon_p = 1 - \sum_i \theta_{si} - \sum_i \theta_{imfi}$$

where θ_{si} and θ_{imfi} are the porosities of the **Solid** and **Immobile Fluids** subnodes under the **Porous Material** node. See Porous Material in the *COMSOL Multiphysics Reference Manual* for more information.

Select **User defined** to enter a value or expression for ε_p.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the porous matrix. The default value is $\chi_p = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Which options are available depends on the **Flow model** setting in the parent node. Note that for the Unsaturated Porous Medium parent node only the Darcian Flow models are available.

Darcian Flow

If **Darcian flow** is selected in the parent **Porous medium** node, select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter** d_p (SI unit: m), the default value is 0.5 mm.

Non-Darcian Flow

If **Non-Darcian flow** is selected in the parent node, select between the following options for the **Permeability model**:

- For **Forchheimer**, the default **Permeability** κ (SI unit: m^2) uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.
- If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm).
- For **Burke–Plummer**, specify the mean **Particle diameter** d_p (default value: 0.5 mm).
- For **Klinkenberg**, the default **Permeability** κ_∞ (SI unit: m^2) uses the value **From material**. Enter the **Klinkenberg parameter** b_K. Its default value is 10^3 Pa.

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Permeability Models in the *Porous Media Flow Module User's Guide*

Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

RETENTION MODEL

For an Unsaturated Porous Medium select between the following options for the retention model:

- **van Genuchten**, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants α (the default value is 1, and the SI unit is $1/\mathrm{m}$), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to $1 - 1/n$.
- **Brooks and Corey** to use the retention model according to the Brooks and Corey relationships.
- **User defined** to use a different retention model. Enter user defined expressions for the **Effective saturation** S_e, the **Liquid volume fraction** θ_l. The default is ε_p (the porosity variable). Specify the **Specific moisture capacity** C_m (SI unit: $1/\mathrm{m}$). The default value is 0 ($1/\mathrm{m}$). Enter an expression for the **Relative permeability** κ_r. The default value is 1.

If there is a residual volume of liquid that cannot move through the pore network, also enter a value between 0 and 1 for the **Residual liquid volume fraction** θ_r. The default value is 0.

Retention and Permeability Relationships in the *Subsurface Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Porous Matrix** node is automatically added to Porous Medium or the Unsaturated Porous Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Fluid**

Richards' Equation > *porous medium feature* > **Fluid**

Unsaturated Porous Medium

The **Unsaturated Porous Medium** node adds Richards' equation (Equation 7-4) for flow in variably saturated porous media.

$$\rho\left(\frac{C_m}{\rho g} + S_e S_p\right)\frac{\partial p}{\partial t} + \nabla \cdot \rho\left(-\frac{\kappa_r \kappa}{\mu}(\nabla p + \rho g \nabla D)\right) = Q_m \qquad (7\text{-}4)$$

The Unsaturated Porous Medium feature has two default subfeatures: the Fluid subfeature, where the fluid density ρ (SI unit: kg/m^3) and viscosity μ (SI unit: Pa·s) are defined, and the Porous Matrix subfeature, where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified as well as the retention model.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Porous Matrix subnode) should be set according to the coordinate system selected in this section.

STORAGE MODEL

With this option, define the first term in Equation 7-4. Therefore, choose from a list one of the following formulations:

- From retention model
- Linearized storage (default)
- From liquid content
- User defined

If **From retention model** is chosen, the first term of Equation 7-4 accounts only for the specific moisture capacity C_m which is defined by the Retention Model in the Porous Matrix subnode:

$$\frac{C_m}{g}\frac{\partial p}{\partial t}.$$

For the option **Linearized storage** the storage coefficient S_p in Equation 7-4 is defined as

$$S_p = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p .$$

From liquid content enforces the first term of Equation 7-4 to be defined in terms of liquid volume fraction as

$$\frac{\partial(\rho\theta_l)}{\partial t}$$

and the **User defined** option allows to define the storage coefficient S_p in Equation 7-4 directly.

Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Unsaturated Porous Medium**
Richards' Equation > **Unsaturated Porous Medium**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Unsaturated Porous Medium**

Dual Porosity Medium

Use the Dual Porosity Medium if the flow through macropores is governed by Darcy's law and the micropores do not significantly contribute to the overall flow in the porous medium.

The feature has three default subfeatures —the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Macropores and Micropores subnodes) should be set according to the coordinate system selected in this section.

STORAGE MODEL

Choose from a list one of the following formulations:

- **From density and porosity** (default), uses the formulation equivalent to Equation 7-1
- **Linearized storage**, where the following linear equation is used to define the storage in the macropores as $S_p = \varepsilon_p\chi_f + (1 - \varepsilon_p)\chi_p$ and in the micropores as $S_{p,m} = \varepsilon_{p,m}\chi_f + (1 - \varepsilon_{p,m})\chi_p$.
- **Poroelastic storage**, where $S_p = \varepsilon_p\chi_f$ in the macropores and $S_{p,m} = \varepsilon_{p,m}\chi_f$ in the micropores.

- **Quasistatic**, where the storage term is set to zero
- **User defined** to directly specify the storage coefficient S_p and $S_{p,m}$ for the macro- and micropores respectively.

- Storage Models in the *Subsurface Flow Module User's Guide*

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, the mass exchange between macro- and microscale system:

$$Q_{ip} = \alpha_w(p_M - p_m) \tag{7-5}$$

with p_M being the pressure within the macropores and p_m the pressure within the micropores.

Find more information in the *Subsurface Flow Module User's Guide*

- Dual Porosity & Dual Permeability Modeling
- Dual Porosity and Dual Permeability Theory

Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Dual Porosity/Permeability** > **Dual Porosity Medium**
Richards' Equation > **Dual Porosity/Permeability** > **Dual Porosity Medium**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Domains > **Dual Porosity/Permeability** > **Dual Porosity Medium**

Dual Permeability Medium

Use the **Dual Permeability Medium** feature to model transport in a saturated dual permeability medium where Darcy's Law describes the transport in each system.

The feature has three default subfeatures —the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Macropores and Micropores subnodes) should be set according to the coordinate system selected in this section.

STORAGE MODEL

With this option under the **Porous Medium** section, Equation 7-1 is formulated with respect to a storage term (analogous to Equation 4-4). Therefore, choose from a list one of the following formulations:

- **From density and porosity** (default), uses the formulation of Equation 4-4
- **Linearized storage**, where the following linear equation is used to define the storage:

$$S_{p,i} = \varepsilon_{p,i}\chi_f + (1 - \varepsilon_{p,i})\chi_{p,i}$$

with i=M for the macropores and i=m for the micropores.

- **Poroelastic storage**, where $S_{p,i} = \varepsilon_{p,i}\chi_f$
- **Quasistatic**, where the storage term is set to zero
- **User defined** to directly specify the storage coefficient S_p

- Storage Models in the *Subsurface Flow Module User's Guide*

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{ip} = \alpha_w(p_M - p_m) \tag{7-6}$$

with p_M being the pressure in the macropores and p_m the pressure in the micropores.

Find more information in the *Subsurface Flow Module User's Guide*

- Dual Porosity & Dual Permeability Modeling
- Dual Porosity and Dual Permeability Theory

Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Dual Porosity/Permeability** > **Dual Permeability Medium**
Richards' Equation > **Dual Porosity/Permeability** > **Dual Permeability Medium**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Domains > **Dual Porosity/Permeability** > **Dual Permeability Medium**

Unsaturated Dual Permeability Medium

Use the **Unsaturated Dual Permeability Medium** feature to model the transport in an unsaturated dual permeability medium where Richards' Equation (Equation 7-4) describes the transport in each system.

$$\begin{gathered}\theta_M\left(\rho\left(S_{e,M}S_{p,M}+\frac{C_{m,M}}{\rho g}\right)\frac{\partial p_M}{\partial t}+\nabla(\rho\mathbf{u}_M)\right)=-Q_{ip}+\theta_M Q_m\\(1-\theta_M)\left(\rho\left(S_{e,m}S_{p,m}+\frac{C_{m,m}}{\rho g}\right)\frac{\partial p_m}{\partial t}+\nabla(\rho\mathbf{u}_m)\right)=Q_{ip}+(1-\theta_M)Q_m\\p=\theta_M p_M+(1-\theta_M)p_m\end{gathered} \tag{7-7}$$

θ_M is the volume fraction of the macropores and Q_{ip} is the interporosity flow, which is the mass transfer from the macroscale to the microscale system. The indices M and m stand for macropores and micropores, respectively.

The feature has three default subfeatures —the Fluid subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Macropores and Micropores subnodes) should be set according to the coordinate system selected in this section.

STORAGE MODEL

With this option, define the first term in Equation 7-7. Therefore, choose from a list one of the following formulations:

- From retention model
- Linearized storage (default)
- From liquid content
- User defined

If **From retention model** is chosen, the first term of Equation 7-7 accounts only for the specific moisture capacity $C_{m,i}$ which is defined by the Retention Model in the Macropores (i=M) or Micropores (i=m) subnode:

$$\frac{C_{mi}}{g}\frac{\partial p}{\partial t}.$$

For the option **Linearized storage** the storage coefficient $S_{p,i}$ in Equation 7-7 is defined as

$$S_{p,i} = \varepsilon_{p,i}\chi_f + (1-\varepsilon_{p,i})\chi_{p,i}.$$

From liquid content enforces the first term of Equation 7-7 to be defined in terms of liquid volume fraction as

$$\frac{\partial(\rho\theta_{l,i})}{\partial t}$$

- and the **User defined** option allows to define the storage coefficient $S_{p,i}$ in Equation 7-7 directly.

- Storage Models in the *Subsurface Flow Module User's Guide*

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{ip} = \alpha_w(p_M - p_m) \tag{7-8}$$

with p_M being the pressure within the macroscale system and p_m the pressure within the microscale system.

- Dual Porosity & Dual Permeability Modeling in the *Subsurface Flow Module User's Guide*

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Dual Porosity/Permeability** > **Unsaturated Dual Permeability Medium**
Richards' Equation > **Dual Porosity/Permeability** > **Unsaturated Dual Permeability Medium**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Domains > **Dual Porosity/Permeability** > **Unsaturated Dual Permeability Medium**

Macropores

This node defines the porosity and material properties of the macroporous matrix of the Dual Porosity Medium, the Dual Permeability Medium, or the Unsaturated Dual Permeability Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

VOLUME FRACTION

Here enter the **Volume Fraction of Macropores**, θ_M.

MATRIX PROPERTIES

The default **Porosity** $\varepsilon_{p,M}$ of the solid matrix of the macropore system is taken **From material**. Select **User defined** to enter a value or expression for $\varepsilon_{p,M}$.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the porous matrix of the macropore system. The default value is $\chi_{p,M} = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. For the macropore settings only the Darcian Flow models are available. Select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability** κ_M (SI unit: m^2) uses the value **From material**, as defined by the **Porous material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K_M (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter** $d_{p,M}$ (SI unit: m), the default value is 0.5 mm.

RETENTION MODEL

For an Unsaturated Dual Permeability Medium select between the following options for the retention model:

- **van Genuchten**, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants α (the default value is 1, and the SI unit is 1/m), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to $1 - 1/n$.

- **Brooks and Corey** to use the retention model according to the Brooks and Corey relationships.
- **User defined** to use a different retention model. Enter user defined expressions for the **Effective saturation** $S_{e,M}$, the **Liquid volume fraction** $\theta_{l,M}$. The default is $\varepsilon_{p,M}$ (the porosity variable). Specify the **Specific moisture capacity** $C_{m,M}$ (SI unit: $1/m$). The default value is 0 ($1/m$). Enter an expression for the **Relative permeability** $\kappa_{r,M}$. The default value is 1.

If there is a residual volume of liquid that cannot move through the pore network, also enter a value between 0 and 1 for the **Residual liquid volume fraction** θ_r. The default value is 0.

Retention and Permeability Relationships in the *Subsurface Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Macropores** node is automatically added to the Dual Porosity Medium, the Dual Permeability Medium, and the Unsaturated Dual Permeability Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Macropores**
Richards' Equation > *porous medium feature* > **Macropores**

Micropores

This node defines the porosity and material properties of the microporous matrix of the Dual Porosity Medium, Dual Permeability Medium, or the Unsaturated Dual Permeability Medium parent node.

MODEL INPUT

This section is only available for the Unsaturated Dual Permeability Medium parent node and contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The default **Porosity** $\varepsilon_{p,m}$ of the solid matrix of the micropore system is taken **From material**. Select **User defined** to enter a value or expression for $\varepsilon_{p,m}$.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the microscale porous matrix. The default value is $\chi_{p,m} = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity to transmit flow for the porous material of the microscale system. Here, only the Darcian Flow models are available. Select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability** κ_m (SI unit: m^2) uses the value **From material**, as defined by the **Porous material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K_m (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter** $d_{p,m}$ (SI unit: m), the default value is 0.5 mm.

RETENTION MODEL

For an Unsaturated Dual Permeability Medium select between the following options for the retention model:

- **From macropores** to take over the retention model settings from the **Macropores** node.
- **van Genuchten**, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants α (the default value is 1, and the SI unit is 1/m), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to $1 - 1/n$.
- **Brooks and Corey** to use the retention model according to the Brooks and Corey relationships.
- **User defined** to use a different retention model. Enter user defined expressions for the **Effective saturation** $S_{e,m}$, the **Liquid volume fraction** $\theta_{l,m}$. The default is $\varepsilon_{p,m}$ (the porosity variable). Specify the **Specific moisture capacity** $C_{m,m}$ (SI unit: 1/m). The default value is 0 (1/m). Enter an expression for the **Relative permeability** $\kappa_{r,m}$. The default value is 1.

If there is a residual volume of liquid that cannot move through the pore network, also enter a value between 0 and 1 for the **Residual liquid volume fraction** θ_r. The default value is 0.

	Retention and Permeability Relationships in the *Subsurface Flow Module User's Guide*

INITIAL VALUES

Define the initial pressure of the microscale system. The default is to use the initial values defined in the Initial Values feature node which means that the same initial values apply to the macroscale and the microscale system.

Select **User Defined** to specify an initial pressure for the microscale system $p_{m0,init}$.

	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

LOCATION IN USER INTERFACE

A default **Micropores** node is automatically added to the Dual Porosity Medium, the Dual Permeability Medium, and the Unsaturated Dual Permeability Medium node.

Context Menus

Darcy's Law > *porous medium feature* > **Micropores**
Richards' Equation > *porous medium feature* > **Micropores**

Mass Source

The **Mass Source** node adds a mass source Q_m, which appears on the right-hand side of the Darcy's Law equation (Equation 7-1).

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{7-9}$$

For the Fracture Flow interface, the mass source is applicable to the right-hand side of Equation 4-40 in the *Subsurface Flow Module User's Guide* (where it is multiplied with the fracture thickness).

MASS SOURCE

Enter a value or expression for the **Mass source** Q_m (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Mass Source**
Richards' Equation > **Mass Source**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Mass Source**

Contributing Velocity

The **Contributing Velocity** node adds a velocity contribution $\mathbf{u}_{ctrb}$ to the velocity field $\mathbf{u}_d$ that is computed from the flow model selected in the parent Porous Medium, Unsaturated Porous Medium, or Dual Porosity Medium feature. The total velocity field used in the continuity equation is therefore

$$\mathbf{u} = \mathbf{u}_d + \mathbf{u}_{ctrb} \tag{7-10}$$

Such velocity contributions can arise in multiphysics models that involve, for example, transport of solutes. If several **Contributing Velocity** nodes are added under the same parent feature, the contributions are treated additively. The sum of all contributing velocity fields is available in the variables `name.Uctrb` (material frame) and `name.uctrb` (spatial frame), with `name` being the **Name** of the physics interface (for example, `dl`).

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list to specify the coordinate system in which the contributing velocity field is given. The default is the **Global coordinate system**. Note that the coordinate system used to specify the components of the contributing velocity field can be selected independently of the coordinate system of the parent feature.

CONTRIBUTING VELOCITY

The default contributing velocity field $\mathbf{u}_{\text{ctrb}}$ is **User defined**, which lets you enter the components of the contributing velocity field explicitly. If a matching velocity field is announced by another feature, it will be available in the selection list.

ADVANCED

Select the **Frame** in which the contributing velocity field is specified. The default is the **Reference configuration**, which means that the velocity field follows the material under, for example, a rotation of the domain. If instead your contributing velocity field follows a fixed direction in space, select the **Deformed configuration**. This section is only displayed if **Advanced Physics Options** is activated and the spatial and material frame of the component differ, such as in the presence of a **Moving Mesh** or **Solid Mechanics** interface.

LOCATION IN USER INTERFACE

Context Menus

If the selected *porous medium feature* is Porous Medium, Unsaturated Porous Medium, or Dual Porosity Medium:

Darcy's Law > *porous medium feature* > **Contributing Velocity**
Richards' Equation > *porous medium feature* > **Contributing Velocity**

Ribbon

Physics tab with **Porous Medium**, **Unsaturated Porous Medium**, or **Dual Porosity Medium** selected:

Attributes > **Contributing Velocity**

Initial Values

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

If you have the Subsurface Flow Module licensed, you can specify the pressure either directly or as an expression for the pressure head, H_p, or the hydraulic head, H; the hydraulic head and the pressure head relate to the pressure p as

$$H_p = \frac{p}{\rho g}; \quad H = H_p + D$$

where ρ is the fluid density (SI unit: kg/m^3); g denotes the acceleration of gravity (SI unit: m/s^2); and D is the elevation (SI unit: m).

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa.

In case the Subsurface Flow Module is available, click the **Pressure head** button to enter a value or expression for H_p (SI unit: m). The default is 0 m. Click the **Hydraulic head** button to enter a value or expression for H (SI unit: m). The default is 0 m.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Initial Values**
Richards' Equation > **Initial Values**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Initial Values**

Gravity

The **Gravity** node is automatically added when **Include gravity** is selected at interface level in the **Darcy's Law** settings and it is active in all domains in which the Darcy's Law interface is applied.

COORDINATE SYSTEM SELECTION

The **Global coordinate system** is selected by default. The **Coordinate system** list contains any additional coordinate systems that the model includes. It can be used when prescribing the direction of the gravitational forces.

GRAVITY

Specify either the acceleration vector or — in case you have a Subsurface Flow Module license — the elevation.

When **Acceleration** is selected from the list, enter the components of the **Gravity vector g**. The default value is `g_const` which is the physical constant having the value 9.8066 $\mathrm{m/s^2}$.

- For 3D and 2D axisymmetric models, the default value is `-g_const` in the z direction.
- For 2D models, the default value is `-g_const` in the y direction.

When **Elevation** is selected from the list, specify the **Elevation** D (SI unit: m). The **Acceleration of gravity** is taken **From physics interface** by default but could be overridden when **User defined** is selected.

When the checkbox **Include gravity** is not selected in the Darcy's Law interface Settings, the elevation D is set equal to zero.

Select the checkbox **Specify reference position** to define a reference position for the gravity calculation.

LOCATION IN USER INTERFACE

Context Menus
Darcy's Law > **Gravity**
Richards' Equation > **Gravity**

Cross Section

Use this node with 1D components to model domains with another cross-sectional area than the global one that is used in the interface **Physical Model** section. In 1D geometries, the pressure is assumed to be constant in the radial direction, and Darcy's Law accounts for that.

CROSS SECTION

Enter values for the **Cross-sectional area** A_c to set the cross section of the domain in the plane perpendicular to the 1D geometry.

LOCATION IN USER INTERFACE

Context Menus
Darcy's Law > **Cross Section**
Richards' Equation > **Cross Section**

Ribbon
Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Cross Section**

Thickness

Use this node with 2D and 1D axisymmetric components to model domains with another thickness than the overall thickness that is specified in the interface **Physical Model** section. In 2D geometries, the pressure is assumed to be constant in the out-of-plane direction (the z direction with default spatial coordinate names). In 1D axisymmetric geometries the thickness represents the z direction.

THICKNESS

Specify a value for the **Thickness** d_z of the domain in the out-of-plane direction. This value replaces the overall thickness in the domains that are selected in the **Domain Selection** section, and is used to multiply some terms into the heat equation.

LOCATION IN USER INTERFACE

Context Menus
Darcy's Law > **Thickness**
Richards' Equation > **Thickness**

Ribbon
Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Thickness**

Porous Electrode Coupling

Use the **Porous Electrode Coupling** node to define a mass source based on the volumetric current densities of one or multiple **Porous Electrode Reaction** nodes in an Electrochemistry interface.

The source (or sink) is proportional to the **Molar mass (kg/mol)** of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

SPECIES

Based on the number of species required for the model, use the **Add** (+) and **Delete**) buttons under the table to add or remove **Species**. Then enter a value for the **Molar mass (kg/mol)** in the applicable rows for each species.

The setting in the table will determine the number of available fields for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Porous Electrode Coupling**
Richards' Equation > **Porous Electrode Coupling**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Domains > *interface* > **Porous Electrode Coupling**

Electrode Surface Coupling

Use the **Electrode Surface Coupling** node to define a combined wall and inflow/outflow boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flow is proportional to the **Molar mass (kg/mol)** of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

SPECIES

Based on the number of species required for the model, use the **Add** (+) and **Delete**) buttons under the table to add or remove **Species**. Then enter a value for the **Molar mass (kg/mol)** in the applicable rows for each species.

The setting in the table will determine the number of available field for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Electrode Surface Coupling**
Richards' Equation > **Electrode Surface Coupling**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Electrode Surface Coupling**

Pressure

Use the **Pressure** node to specify the pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example.

PAIR SELECTION

If this node is selected from the **Pairs** menu, choose the pair to apply this condition to. A pair must be created first. See Identity, Contact, and Sector Symmetry Pairs in the *COMSOL Multiphysics Reference Manual* for more details.

PRESSURE

Enter a value or expression for the **Pressure** p_0 (SI unit: Pa). Enter a relative pressure value in p_0 (SI unit: Pa).

For the Subsurface Flow Module, the **Pressure** node provides the pressure P_0 as a condition on edges in 3D models. Then select the edges under **Edge Selection**.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

As an attribute to the Fracture boundary condition or as boundary condition to The Fracture Flow Interface (which are available in the Subsurface Flow Module and the Porous Media Flow Module), the pressure can also be specified on edges (in 3D) or points (in 2D) surrounding the fracture domain. In other cases, pressure constraints on edges or points are not implemented.

!	If the boundary condition is adjacent to an Unsaturated Dual Permeability Medium feature it constrains the pressures in the Macropores and Micropores to p_0.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Pressure**
Richards' Equation > **Pressure**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Pressure**
Pairs > *interface* > **Pressure**

Mass Flux

Use the **Mass Flux** node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n} \cdot \rho\frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0. A positive value of N_0 represents an inward mass flux whereas a negative value represents an outward mass flux. The units are based on the geometric entity: **Boundaries**: (SI unit: kg/(m^2·s)).

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Mass Flux**
Richards' Equation > **Mass Flux**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Mass Flux**

Line Mass Source

The **Line Mass Source** node adds mass flow originating from a tube of infinitely small radius.

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the symmetry axis
3D	Edges

LINE MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(m·s)). A positive value results in mass injection from the line into the computational domain, and a negative value means that the mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

Fracture Flow

The equivalent feature available for fracture flow is the **Mass Source** attribute of the Fracture boundary condition and the **Mass Source** point feature of the Fracture Flow Interface, both available in 3D only.

LOCATION IN USER INTERFACE

According to the model dimension as mentioned in Selection, this feature is available for the *geometrical entities* **Edges** or **Points**.

Context Menus

Darcy's Law > *geometrical entity* > **Line Mass Source**
Richards' Equation > *geometrical entity* > **Line Mass Source**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

geometrical entity > **Line Mass Source**

Point Mass Source

The **Point Mass Source** node models mass flow originating from an infinitely small sphere centered around a point. It is available for points in 3D geometries.

POINT MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(s)). A positive value results in mass injection from the point into the computational domain, and a negative value means that the mass is removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Points** > **Point Mass Source**
Richards' Equation > **Points** > **Point Mass Source**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Points > **Point Mass Source**

Inlet

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary. It has three options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity. A negative value represents an outflow velocity. The inlet velocity boundary condition is implemented as;

$$\mathbf{n} \cdot \rho\frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) = \rho U_0$$

where U_0 is a value or expression for the specified inward (or outward) Darcy velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas

a negative value represents an outflow. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

PRESSURE

Use the **Pressure** option to specify the inlet pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example. Enter a value or expression for the **Pressure** p_0 (SI unit: Pa).

MASS FLOW

If you select **Mass flow** as the inlet condition, specify the total **Mass flow rate** M_0 (SI unit: kg/s), or the **Pointwise mass flux** N_0 (SI unit: kg/(m^2·s)).

With **Mass flow rate** boundary condition, positive values correspond to flow into the model domain:

$$-\int_{\partial\Omega} \rho(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S = M_0$$

where M_0 is a value or expression for the specified inward (or outward) Darcy flux.

Pointwise mass flux boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n}\cdot\rho\frac{\kappa}{\mu}(\nabla p + \rho g\nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Inlet**
Richards' Equation > **Inlet**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Inlet**

Symmetry

The **Symmetry** node describes a symmetry boundary. The following condition implements the symmetry condition on an axis or a flow divide:

$$\mathbf{n} \cdot \frac{\kappa}{\mu} \nabla p = 0$$

$$\mathbf{n} \cdot \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Symmetry**
Richards' Equation > **Symmetry**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Symmetry**

No Flow

The **No Flow** node is the default boundary condition stating that there is no flow across impermeable boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

where $\mathbf{n}$ is the vector normal to the boundary. D is the elevation head which is set to zero for any other than Subsurface Flow Module applications.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **No Flow**
Richards' Equation > **No Flow**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **No Flow**

Flux Discontinuity

Use the **Flux Discontinuity** node to specify a mass flux discontinuity through an interior boundary. The condition is represented by the following equation:

$$-\mathbf{n} \cdot (\rho \mathbf{u}_1 - \rho \mathbf{u}_2) = N_0$$

In this equation, $\mathbf{n}$ is the vector normal (perpendicular) to the interior boundary, ρ is the fluid density, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the Darcy velocities in the adjacent domains (as defined in Equation 7-11) and N_0 is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{7-11}$$

For this boundary condition, a positive value of N_0 corresponds to a flow discontinuity in the opposite direction to the normal vector of the interior boundary.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: kg/(m^2·s)). A positive value of N_0 represents a mass flux discontinuity in the opposite direction to the normal vector of the interior boundary.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Interior Surfaces** > **Flux Discontinuity**

Richards' Equation > **Interior Surfaces** > **Flux Discontinuity**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Interior Surfaces** > **Flux Discontinuity**

Pairs > **Flux Discontinuity**

Outlet

The **Outlet** node adds a boundary condition for the outflow (or inflow) perpendicular (normal) to the boundary. It has different options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal outflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an outflow velocity whereas a negative value represents an inflow velocity.

$$-\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = \rho U_0$$

where U_0 is a specified value or expression for the outward (or inward) Darcy velocity.

PRESSURE

Similar to the inlet **Pressure** option, the outlet pressure on a boundary can be specified. Enter a value or expression for the **Pressure** p_0 (SI unit: Pa).

DISCHARGE

Enter a value or expression for the discharge Q_D to specify the volumetric flow rate through the boundary. The mass flux $\rho\mathbf{u}$ is related to the discharge as follows:

$$\int_{\partial\Omega} \rho\mathbf{u} \cdot \mathbf{ds} = \rho Q_D \,. \tag{7-12}$$

The mean normal outflow velocity at the boundary can then be calculated as $U_\mathrm{out} = Q_\mathrm{D}/A$, where A is the cross sectional area of the boundary.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Outlet**

Richards' Equation > **Outlet**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equation** selected:

Boundaries > *interface* > **Outlet**

Precipitation

The **Precipitation** node adds a boundary condition for the inflow (of rain) perpendicular (normal) to the boundary.

Enter a value or expression for the **Precipitation rate** which then contributes to the mass flux at the selected boundaries.

Select the **Slope correction** checkbox to apply a correction that depends on the normal to the boundary and the vertical axis. This is needed when the boundary is inclined.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Precipitation**
Richards' Equation > **Hydraulics** > **Precipitation**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Precipitation**

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries. It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of velocity and pressure across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Interior Surfaces** > **Interior Wall**
Richards' Equation > **Interior Surfaces** > **Interior Wall**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Interior Surfaces** > **Interior Wall**

Thin Barrier

The **Thin Barrier** boundary condition models interior permeable walls, membranes, geotextiles, or perforated plates as thin permeable barriers. The **Thin Barrier** boundary condition can only be applied on interior boundaries.

WALL

Enter a value or expression for the **Thickness** d_b (SI unit: m, the default is 0.1 m) and for the **Permeability** κ_b (SI unit: m^2). The default **Permeability** κ_b uses the value **From material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Full** to define a tensor value and enter another value or expression in the field or matrix.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Interior Surfaces** > **Thin Barrier**
Richards' Equation > **Interior Surfaces** > **Thin Barrier**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Interior Surfaces** > **Thin Barrier**

Pressure Head

Use the **Pressure Head** node to specify the pressure head (instead of the pressure) on a boundary. It adds this boundary condition for the pressure head $H_p = H_{p0}$, where H_{p0} is a known pressure head given as a number, a distribution, or an expression involving time, t, for example. The dimension of the pressure head is length (SI unit: m).

PRESSURE HEAD

Enter a value or expression for the **Pressure head** H_{p0} (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Pressure Head**
Richards' Equation > **Hydraulics** > **Pressure Head**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Pressure Head**
Pairs > **Pressure Head**

Hydraulic Head

Use the **Hydraulic Head** node to specify the hydraulic head (instead of the pressure) on a boundary. This adds the Dirichlet condition for the hydraulic head $H = H_0$ where H_0 is a known hydraulic head given as a number, a distribution, or an expression involving time, t, for example.

HYDRAULIC HEAD

Enter a value or expression for the **Hydraulic head** H_0 (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Hydraulic Head**
Richards' Equation > **Hydraulics** > **Hydraulic Head**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Hydraulic Head**
Pairs > **Hydraulic Head**

Atmosphere/Gauge

The **Atmosphere/Gauge** node specifies an atmospheric pressure or gauges the pressure to the atmospheric value. This means that the total hydraulic potential reduces to the

gravitational pressure at the free surface. At a free surface, such as a spring or a seepage face, the pressure is atmospheric. If the pressures in the model is gauged to the atmospheric value ($p = 0$), the total hydraulic potential reduces to the gravitational potential at the free surface — for example, the height of the free surface multiplied by the fluid weight, or $\rho_f g D$. This boundary condition sets the pressure at the boundary to zero and $p = 0$.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Atmosphere/Gauge**
Richards' Equation > **Hydraulics** > **Atmosphere/Gauge**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Atmosphere/Gauge**

Pervious Layer

The **Pervious Layer** node provides a boundary condition that describes a mass flux through a semi-pervious layer connected to an external fluid source at different pressure, pressure head, or hydraulic head. The model domain might connect to a larger body of water through the semi-pervious layer. This condition is represented with the following boundary condition:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) = \rho R_b \left[\frac{(p_b - p)}{\rho g} + (D_b - D) \right] \tag{7-13}$$

In this equation, p_b (SI unit: Pa) and D_b (SI unit: m) are the pressure and the elevation of the distant fluid source, respectively, and R_b (SI unit: 1/s) is the conductance of materials between the source and the model domain (conductance to flow in the semi-pervious layer adjacent to the boundary). Typically $R_b = K'/B'$, where K' is the hydraulic conductivity (SI unit: m/s) of the layer and B' (SI unit: m) is its thickness. Using logical relationships, it is possible to activate these expressions at different times or under various flow conditions.

When the pressure head H_p is specified instead of the pressure, the boundary condition is the following:

$$\mathbf{n} \cdot \rho K \nabla (H_p + D) = \rho R_b [(H_{pb} - H_p) + (D_b - D)] \quad (7\text{-}14)$$

H_{pb} is the pressure head (SI unit: m) at the edge of the layer.

When the hydraulic head H is specified instead of the pressure head, the boundary condition becomes:

$$\mathbf{n} \cdot \rho K \nabla H = \rho R_b [H_b - H] \quad (7\text{-}15)$$

H_b is the hydraulic head (SI unit: m) at the edge of the layer.

K in Equation 7-14 and Equation 7-15 is the hydraulic conductivity.

At a free surface, such as a water table or seepage face, the pressure is atmospheric (here taken to be zero), so the total hydraulic potential equals gravitational potential, which is defined on D.

Gravity effects are not active by default. Select the checkbox **Include gravity** to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

PERVIOUS LAYER

Specify the material properties whether to specify an external pressure, pressure head, or hydraulic head.

Select an **External variable to specify** — **Pressure and elevation** to specify the external pressure, **Pressure head and elevation** to specify the external pressure head, or **Hydraulic head**. For all selections, enter a value for the **Conductance** R_b (SI unit: 1/s).

- For **Pressure and elevation** enter an **External pressure** p_b (SI unit: Pa) and **External elevation** D_b (SI unit: m).
- For **Pressure head and elevation** enter an **External pressure head** H_{pb} (SI unit: m), H_{pb} (SI unit: m) and **External elevation** D_b (SI unit: m).
- For **Hydraulic head** enter the **Hydraulic head** H_b (SI unit: m).

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Hydraulics** > **Pervious Layer**

Richards' Equation > **Hydraulics** > **Pervious Layer**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

Boundaries > **Hydraulics** > **Pervious Layer**

Well

The **Well** feature is intended to model injection or production wells and is available with the Subsurface Flow Module.

WELL

Enter a value or expression for the **Well diameter** d_w (SI unit: m, the default is 0.1 m). Select the **Well type** from the list: **Production** or **Injection**.

Specify either the **Pressure** (SI unit: Pa), **Pressure head** (SI unit: m), **Hydraulic head** (SI unit: m), or the **Mass flow**. If you select **Mass flow**, specify the total **Mass flow rate** (SI unit: kg/s), the **Mass flow rate per unit length** (SI unit: kg/(m·s)) or the **Mass flux** (SI unit: kg/(m^2·s)).

LOCATION IN USER INTERFACE

According to the model dimension this feature is available for the *geometrical entities* **Edges** (3D) or **Points** (2D).

Context Menus

Darcy's Law > *geometrical entity* > **Well**
Richards' Equation > *geometrical entity* > **Well**

Ribbon

Physics tab with **Darcy's Law** or **Richards' Equation** selected:

geometrical entity > **Well**

Fracture

Use the **Fracture** node to model flow along a boundaries representing fractures within a porous medium. By default, it adds the tangential form of the continuity equation and of Darcy's Law.

$$d_f \frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla_T \cdot (d_f \rho \mathbf{u}) = d_f Q_m \tag{7-16}$$

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla_T p \tag{7-17}$$

The **Fracture** feature has two default subfeatures — the Fluid (Fracture) subfeature where the fluid density ρ (SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Fracture Material subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or **Hydraulic conductivity** (in the Fracture Material subnode) should be set according to the coordinate system selected in this section.

APERTURE

Enter a value for the **Fracture thickness** d_f.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship using Equation 7-16 and Equation 7-17.
- **Non-Darcian flow** defines a nonlinear relationship using Equation 7-16 and the pressure-velocity relationship

$$\nabla_T p = -\frac{\mu}{\kappa}\mathbf{u} - \beta\rho|\mathbf{u}|\mathbf{u}$$

  where the nonlinear parameter β (SI unit: $1/m$) is further specified in the Fracture Material subfeature.

STORAGE MODEL

Equation 7-16 can also be formulated with respect to a storage term.

$$\rho S\frac{\partial p}{\partial t} + \nabla \cdot \rho\left[-\frac{\kappa}{\mu}(\nabla p)\right] = Q_m$$

The storage coefficient S can be interpreted as the weighted compressibility of the porous material and the fluid. Define the time dependent storage term by selecting one of the following options from the list:

- **From density and porosity** (default), uses the formulation of Equation 7-16
- **Linearized storage**, where the following linear equation is used to define the storage:

$$S = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p$$

- **User defined** to directly specify the storage coefficient S

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Storage Models in the *Subsurface Flow Module User's Guide*

FRACTURE MODEL

Choose between two options to model fractures that have different characteristics.

- **Highly conductive fracture** represents a fracture filled with a highly permeable material.
- **Thin conducting barrier** represents a fracture that is filled with a low permeable material and therefore acts as a barrier for the flow which adds a jump in the pressure across the boundary:

$$-\mathbf{n}_{u,d} \cdot (\rho \mathbf{u})_{u,d} = \rho \frac{(p_{d,u} - p_{u,d})}{d_b} \frac{\kappa_b}{\mu}$$

The barrier thickness d_b and permeability κ_b are defined in the Fracture Material subnode.

In addition, either on the upside, downside, or on both sides a highly conductive fracture material is present and Equation 7-16 and Equation 7-17 are solved for the highly conductive side. Further specifications are done in the Fracture Material subnode.

Note that the option to specify the **Fracture Model** is only available for the Fracture feature within the Darcy's Law interface.

For the Fracture boundary node several subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. As they are

almost identical to the boundary conditions of the Fracture Flow interface, see Domain, Boundary, Edge, Point, and Pair Nodes for the Fracture Flow Interface in the *Subsurface Flow User's Guide* for further description. Note that **Precipitation** is only available for the Fracture Flow interface.

This feature requires a specific license. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

Flow in a Fractured Reservoir: Application Library path **Subsurface_Flow_Module/Fluid_Flow/fractured_reservoir_flow**

LOCATION IN USER INTERFACE

Context Menus

Darcy's Law > **Fracture**
Richards' Equation > **Fracture**
Fracture Flow > **Fracture**

Ribbon

Physics tab with *interface* as **Darcy's Law** or **Richards' Equations** selected:

Boundaries > *interface* > **Fracture**

With **Fracture Flow** selected:

Boundaries > **Fracture**

Fluid (Fracture)

This node defines the material properties of the fluid of the Fracture parent node. The fluid can be specified as general gas or liquid or as an ideal gas.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

The available options for the **Fluid type** are **Gas/Liquid** (default) or **Ideal gas**. The selection determines how the density and compressibility of the fluid are set. The latter is only required if a linearized storage model has been selected in the parent Fracture node. For all fluid types specify the dynamic viscosity μ (SI unit: Pa·s).

Gas/Liquid

This option specifies the **Density** and the **Compressibility** for a general gas or liquid.

Ideal Gas

For **Ideal gas** it uses the ideal gas law to describe the fluid. In this case, specify the thermodynamics properties. Select a **Gas constant type** — **Specific gas constant** R_s (the default) or **Mean molar mass** M_n (SI unit: J/(mol·K)). For **Mean molar mass** the universal gas constant $R = 8.314$ J/(mol·K) is used as the built-in physical constant. For both properties, the defaults use values **From material**. For **User defined** enter another value or expression.

If required by a **Storage Model**, the **Compressibility** of the ideal gas is calculated as $\chi_f = 1/p_A$ with the absolute pressure p_A (Pa).

If **Hydraulic conductivity** is selected as the **Permeability model** (see the Fracture Material section), dynamic viscosity is not available. The hydraulic conductivity is defined using a combination of fluid and fracture material properties and replaces the need of defining the dynamic viscosity.

LOCATION IN USER INTERFACE

A default **Fluid** node is automatically added to the Fracture node.

Context Menus

Darcy's Law > **Fracture** > **Fluid**
Richards' Equation > **Fracture** > **Fluid**
Fracture Flow > **Fracture** > **Fluid**

Fracture Material

This node defines the porosity and material properties of the solid matrix of the Fracture parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

BARRIER PROPERTIES

This section appears if the **Thin conducting barrier** option for the **Fracture model** is chosen in the parent Fracture feature.

Enter the values for the barrier thickness d_b and permeability κ_b.

Note that the **Thin Conductive barrier** option is only available for the Fracture feature within the Darcy's Law interface.

FRACTURE MATERIAL PROPERTIES

If the **Thin conducting barrier** option for the **Fracture model** is chosen in the parent Fracture feature you can specify the **Conductive layer position** here. Choose between **Both sides**, **Upside**, and **Downside**. A sketch above shows the position of conductive layers and barrier within the fracture.

The **Porosity** ε_p of the fracture material is taken **From material** by default. Select **User defined** to enter a value or expression for ε_p.

If required by a **Storage model** in the parent node, specify the **Effective compressibility** of the porous matrix. The default value is $\chi_p = 10^{-4}$ 1/Pa.

Select a **Permeability model** to specify the capacity of the fracture material to transmit flow. Which options are available depends on the **Flow model** setting in the parent node.

- Select **Permeability** (default) to define the permeability of the fracture material.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For **Hydraulic conductivity** K (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Cubic law** to define the permeability from the fracture thickness specified in the parent node and the roughness factor f_f.

If the Non-Darcian Flow Model is selected in the parent Fracture feature enter a value for the **Inertial resistance coefficient** β.

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Permeability Models in the *Porous Media Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Fracture Material** node is automatically added to the Fracture node.

Context Menus

Darcy's Law > **Fracture** > **Fracture Material**
Richards' Equation > **Fracture** > **Fracture Material**
Fracture Flow > **Fracture** > **Fracture Material**

The Brinkman Equations Interface

The **Brinkman Equations (br)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. The physics interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier–Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. To simplify the equations, select the Stokes–Brinkman flow feature to reduce the dependence on inertial effects when the Reynolds number is significantly less than 1. The physics interface can be used for stationary and time-dependent analyses.

The main node is the Porous Medium feature, which adds the Brinkman equations and provides interfaces for defining the fluid material and the porous matrix.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Porous Medium**, **Wall** (the default boundary type, using **No slip** as the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Brinkman Equations** to select physics features from the context menu.

The boundary conditions are essentially the same as for the Laminar Flow interface. Differences exist for the following boundary types: Outlet, Symmetry, Open Boundary, and Boundary Stress where the viscous part of the stress is divided by the porosity to appear as

$$\frac{1}{\varepsilon_p}\left\{\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}$$

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings**, all accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `br`.

PHYSICAL MODEL

This node specifies the properties of the Brinkman Equations interface, which describe the overall type of fluid flow model.

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Brinkman equations to model constant density flow. Alternatively, from the **Compressibility** list select **Weakly compressible flow**, which should be used when the pressure dependency of the density can be neglected, or **Compressible flow (Ma<0.3)** to solve for the full compressible flow of which, however, the Mach number must be below 0.3.

Swirl Flow

For 2D axisymmetric models, select the **Swirl flow** checkbox to include the swirl velocity component, that is the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction.

Note that this feature is only available for specific modules. See https://www.comsol.com/products/specifications/ for a detailed overview.

Neglect Inertial Term (Stokes–Brinkman Flow)

The **Neglect inertial term (Stokes–Brinkman)** checkbox is selected by default to model flow at low Reynolds numbers for which the inertial term can be neglected. This results in the linear Stokes–Brinkman equations.

Include Gravity

Gravity is not included by default. Select the **Include gravity** checkbox to activate the acceleration of gravity. This automatically adds a global **Gravity** feature node to the interface model tree, and the buoyancy force is included in the equations.

Also, when the **Include gravity** checkbox is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes

are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Porous Treatment of No Slip Condition

Choose how the **No Slip** condition on **Wall** boundaries and **Interior Wall** boundaries adjacent to **Porous Medium** should be treated. The options are **Standard no slip formulation** and **Porous slip** (the default). The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces section.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

Reference Temperature Level

Enter a **Reference temperature level** T_{ref} (SI unit: K). The default value is `293.15[K]`.

Reference Position

If **Include gravity** is selected, a **Reference position** r_{ref} (SI unit: m) can be specified which is then used for the calculation of the hydrostatic pressure.

TURBULENCE

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM** (Reynolds-Averaged Navier–Stokes, eddy-viscosity model) or to **RANS-RSM** (Reynolds-Averaged Navier–Stokes, Reynolds stress model). If **RANS-EVM** is activated, you can set the **Turbulence model** either to one of the algebraic turbulence models, **Algebraic yPlus** (the default) or **L-VEL**, or to one of the following two-equation turbulence models: k-ε, Realizable k-ε, Low Reynolds Number k-ε, k-ω, SST, and v2-f. The **Wall treatment** is set to **Automatic** (default) or **Low Re** while **Wall functions** is available for k-ω and is the only option for k-ε and Realizable k-ε. If **RANS-RSM** is activated, you can set the **Turbulence model** to one of the following seven-equation turbulence models: Wilcox R-ω and SSG-LRR. The **Wall treatment** is **Low Re**.

For more information about turbulence modeling, see Theory for the Turbulent Flow Interfaces in the *CFD Module User's Guide*.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. When selected, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

- Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface
- Theory for the Brinkman Equations Interface
- Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Nitsche Constraints

Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface

The Brinkman Equations Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

These nodes are described in this section:

- Porous Medium
- Initial Values
- Mass Source
- Volume Force
- Fluid Properties

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface :

- Flow Continuity
- Inlet
- Line Mass Source
- Boundary Stress
- Outlet
- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Porous Medium

The **Porous Medium** node adds the Brinkman equations: Equation 4-34 and Equation 4-35 (excluding any mass sources). It has two default subfeatures — the Fluid subfeature where the fluid density ρ(SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the **Global coordinate system**, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the Definitions node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** (in the **Porous Matrix** subnode) should be set according to the coordinate system selected in this section.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship characteristic for low Reynolds number laminar flows.
- **Non-Darcian flow** defines a nonlinear relationship due to inertial or turbulence effects.

POROUS MEDIUM TURBULENCE MODEL

If in the parent feature node a turbulence model other than **Algebraic yPlus** or **L-VEL** is selected, define a model which complements the basic turbulence model and accounts for the influence of the porous matrix on turbulent flow in porous media.

- For **Default** and **Nakayama-Kuwahara** specify the **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} which by default is set to 0.212.
- For **Pedras-de Lemos**, specify the **Choice of the Pedras-de Lemos model coefficient**. When **User defined** is chosen, specify the **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} with default value 0.212. Choosing **Original** results in $C_{stpm} = 0.28 \cdot \sqrt{\varepsilon_p}$, while choosing **Recalibrated** results in $C_{stpm} = 0.18$.
- If **Turbulence model type** is **RANS-RSM**, specify the **Production of Reynolds stresses by porous matrix**. The default is **Isotropic** and the other option is **Streamwise**.

DISTANCE EQUATION

This section is available for the turbulence models **Algebraic yPlus** or **L-VEL**. Select how the **Reference length scale** l_{ref} (SI unit: m) is defined — **Automatic** (default) or **Manual**:

- For Automatic the wall distance is automatically evaluated to one tenth of the shortest side of the geometry bounding box. This is usually quite accurate but it can sometimes give a too high value if the geometry consists of several slim entities. In such cases, define the reference length scale manually.
- For Manual it defines a different value or expression for the length scale. The default is 1 m.

l_{ref} controls the result of the distance equation. Objects that are much smaller than l_{ref} are effectively be diminished while the distance to objects much larger than l_{ref} are accurately represented.

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Porous Medium**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Porous Medium**

Fluid

This node defines the material properties of the fluid of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

Specify the **Density** ρ and the **Dynamic viscosity** μ (SI unit: Pa·s) of the fluid. The defaults use values **From material**, for **User defined** enter a value or expression.

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity.

If the Polymer Flow Module license is available and for Darcian flow, also non-Newtonian models are available and the **Constitutive Relation** can be switched between **Specify dynamic viscosity** (default) or **Inelastic non-Newtonian**.

Constitutive Relation

Use the default option to either get the dynamic viscosity from a material, or to add a user defined expression. The default option lets you either use the dynamic viscosity from a material or define it with a custom expression. The **Inelastic non-Newtonian** option provides several models and defines the **Apparent shear rate**.

Inelastic Non-Newtonian

The following inelastic non-Newtonian Models are available for the **Fluid** feature under the **Porous Medium** feature:

- Power Law

- Carreau
- Carreau-Yasuda
- Cross
- Cross-Williamson
- Sisko

The setup of these models in porous media is similar to their definition under the Fluid Properties feature.

Apparent Shear Rate

To define the apparent shear rate $\dot{\gamma}_{app}$, either enter a user-defined expression for the correction factor (α) or choose the **Capillary bundle approach** from the list and provide a value for the Tortuosity factor (C).

- Read more about the theory of Non-Newtonian Fluids in Porous Media in the *Polymer Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Fluid** node is automatically added to the Porous Medium node.

Context Menus

Brinkman Equations > **Porous Medium** > **Fluid**

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material**. For **User defined** the default value is 1.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Depending on the **Flow model** selection in the parent **Porous Medium** feature node you can choose between the following options:

- **Permeability** (the default) to directly enter the permeability of the porous matrix or **Kozeny-Carman** to define the permeability from the porosity and mean **Particle diameter** for **Darcian** flow or
- **Forchheimer** or **Ergun** for **Non-Darcian** flow.

Note that some of these options are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material** list. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.

For **Kozeny-Carman**, enter the mean **Particle diameter** d_p (SI unit: m), the default value is 0.5 mm.

In case a **Non-Darcian** flow model is chosen in the parent node, **Forchheimer** is the default selection for the **Permeability model**. For **Forchheimer**, the default **Permeability** κ (SI unit: m^2) uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow Module User's Guide*.

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Permeability Models in the *Porous Media Flow Module User's Guide*

LOCATION IN USER INTERFACE

A default **Porous Matrix** node is automatically added to the Porous Medium node.

Context Menus

Brinkman Equations > **Porous Medium** > **Porous Matrix**

Mass Source

The **Mass Source** node adds a mass source (or mass sink) Q_m to the right-hand side of the continuity equation: Equation 7-18. This term accounts for mass deposit and/or mass creation in porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{7-18}$$

DOMAIN SELECTION

Only Porous Matrix domains are available.

MASS SOURCE

Enter a value or expression for the **Source term** Q_{br} (SI unit: kg/(m^3·s)). The default is 0 kg/(m^3·s).

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Mass Source**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Mass Source**

Volume Force

Use the **Volume Force** node to specify the force $\mathbf{F}$ on the right-hand side of Equation 7-19. It then acts on each fluid element in the specified domains.

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) = -\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_m}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F} \tag{7-19}$$

VOLUME FORCE

Enter the components of **Volume force** $\mathbf{F}$ (SI unit: N/m^3).

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Volume Source**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Volume Source**

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Initial Values**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Initial Values**

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations to solve for free flow in nonporous domains. The node also provides an interface for defining the material properties of the fluid.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs — for example, temperature or pressure — may be required to define these properties.

Temperature

By default, the single-phase flow interfaces are set to model isothermal flow. Hence, the **Temperature** is **User defined** and defaults to 293.15 K. If a Heat Transfer interface is included in the component, the temperature may alternatively be selected from this physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p + p_{\text{ref}}$ where p is the dependent pressure variable from the Navier–Stokes equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** ( ) and entering the desired value in the input field.

FLUID PROPERTIES

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible.

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Fluid Properties**

Ribbon

Physics tab with **Brinkman Equations** selected:

Domains > **Fluid Properties**

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value. When a turbulence model that solves for the turbulent kinetic energy, k, is used, the option **Include buoyancy-induced turbulence** is available. When selected, the **Buoyancy contribution** is by default set to **Automatic from multiphysics**. Contributions are only obtained from multiphysics couplings that support buoyancy-induced turbulence, such as Nonisothermal Flow. If the **Buoyancy contribution** is switched to **User defined**, a text field for the **Turbulent Schmidt number** appears. See also Theory for Buoyancy-Induced Turbulence in the *CFD Module User's Guide*.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{const}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{const}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

LOCATION IN USER INTERFACE

Context Menus

Brinkman Equations > **Gravity**

The Free and Porous Media Flow, Brinkman Interface

The **Free and Porous Media Flow, Brinkman (fp)** interface ( ) is found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface. It is used to compute fluid velocity and pressure fields of single-phase flow where free flow is connected to porous media. The Free and Porous Media Flow, Brinkman interface is used over at least two different domains: a free channel and a porous medium. The physics interface is well suited for transitions between slow flow in porous media, governed by the Brinkman equations, and fast flow in channels described by the Navier–Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. The physics interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add a **Porous Medium** node to be used on the domain selection corresponding to the porous media, or add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Free and Porous Media Flow, Brinkman** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `fp`.

PHYSICAL MODEL

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Navier–Stokes and Brinkman equations to model constant density flow. If required, select

Weakly compressible flow from the **Compressibility** list, to account for small variations in the density, which are only dependent on the temperature (nonisothermal flow) or **Compressible flow (Ma<0.3)** for fully compressible flow. However, for the flow modeled with this physics interface, the Mach number must be below 0.3.

Swirl Flow

For 2D axisymmetric components, select the **Swirl flow** checkbox to include the swirl velocity component, that is the velocity component u_φ in the azimuthal direction. While u_φ can be nonzero, there can be no gradients in the φ direction. Note that this feature is only available for specific modules. Visit https://www.comsol.com/products/specifications/ for a detailed overview.

Neglect Inertial Term

Select the **Neglect inertial term (Stokes flow)** checkbox if the inertial forces are small compared to the viscous forces. This is typical for creeping flow, where $\mathrm{Re} << 1$.

Enable porous media domains

The **Enable porous media domains** checkbox is selected by default to solve the Brinkman equations in porous domains. If it is unchecked, the **Porous Medium** node is no longer available in this interface.

Include Gravity

Gravity is not included by default. Select the **Include gravity** checkbox to activate the acceleration of gravity. This automatically adds a global **Gravity** feature node to the interface model tree, and the buoyancy force is included in the Equations.

Also, when the **Include gravity** checkbox is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Porous Treatment of No Slip Condition

Choose how the **No Slip** condition on internal boundaries should be treated. The options are **Standard no slip formulation** and **Porous slip** (default). The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in The Creeping Flow, Laminar Flow, Turbulent Flow, Large Eddy Simulation, and Detached Eddy Simulation Interfaces section.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

Reference Temperature

Enter a **Reference temperature** T_{ref} (SI unit: K). The default value is `293.15[K]`.

Reference Position

If **Include gravity** is selected, a **Reference position** r_{ref} (SI unit: m) can be specified which is then used for the calculation of the hydrostatic pressure.

TURBULENCE

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS-EVM** (Reynolds-Averaged Navier–Stokes, eddy-viscosity model), **RANS-RSM** (Reynolds-Averaged Navier–Stokes, Reynolds stress model), or **Large Eddy Simulation** (which is only available in 3D). If turbulent flow is activated, you can choose from different **Turbulence model**s and options for **Wall treatment**. For a description of the different turbulence models, wall treatment options, and turbulence model parameters, see Theory for the Turbulent Flow Interfaces in the *CFD Module User's Guide*.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

- Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow, Brinkman Interface
- Theory for the Free and Porous Media Flow, Brinkman Interface

Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow, Brinkman Interface

The Free and Porous Media Flow, Brinkman Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid Properties
- Gravity
- Initial Values
- Porous Medium
- Mass Source
- Volume Force
- Wall

Note that some features are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/).

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface:

- No Viscous Stress
- Flow Continuity
- Inlet
- Line Mass Source
- Outlet
- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

Use the **Fluid Properties** node to define the fluid material, density, and dynamic viscosity.

FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

The default **Density** ρ (SI unit: kg/m^3) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 kg/m^3.

The **Dynamic viscosity** μ (SI unit: Pa·s) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

Porous Medium

The **Porous Medium** node adds the Brinkman equations (excluding any mass sources) to the interface. It has two default subfeatures — the Fluid subfeature where the fluid density ρ(SI unit: kg/m^3) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- **Darcian flow** (default) defines a linear relationship characteristic for low Reynolds number laminar flows.
- **Non-Darcian flow** defines a nonlinear relationship due to inertial or turbulence effects.

POROUS MEDIUM TURBULENCE MODEL

Defines a model which complements the basic turbulence model and accounts for the influence of the porous matrix on turbulent flow in Porous Media.

- **Default** and **Nakayama-Kuwahara** specify **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} which by default is set to 0.212.
- **Pedras-de Lemos** asks to specify **Choice of the Pedras-de Lemos model coefficient**. When **User defined** is chosen, specify **Coefficient of subgrid turbulence generation by porous matrix** C_{stpm} with default value 0.212. Choosing **Original** results in $C_{stpm} = 0.28 \cdot \sqrt{\varepsilon_p}$, while choosing **Recalibrated** results in $C_{stpm} = 0.18$.

Fluid

This node defines the material properties of the fluid of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

Specify the **Density** ρ and the **Dynamic viscosity** μ (SI unit: Pa·s) of the fluid. The defaults use values **From material**, for **User defined** enter a value or expression.

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity.

If the Polymer Flow Module license is available and for Darcian flow, also non-Newtonian models are available and the **Constitutive Relation** can be switched between **Specify dynamic viscosity** (default) or **Inelastic non-Newtonian**.

Constitutive Relation

Use the default option to either get the dynamic viscosity from a material, or to add a user defined expression. The default option lets you either use the dynamic viscosity from a material or define it with a custom expression. The **Inelastic non-Newtonian** option provides several models and defines the **Apparent shear rate**.

Inelastic Non-Newtonian

The following inelastic non-Newtonian Models are available for the **Fluid** feature under the **Porous Medium** feature:

- Power Law
- Carreau
- Carreau-Yasuda
- Cross
- Cross-Williamson
- Sisko

The setup of these models in porous media is similar to their definition under the Fluid Properties feature.

Apparent Shear Rate

To define the apparent shear rate $\dot{\gamma}_{app}$, either enter a user-defined expression for the correction factor (α) or choose the **Capillary bundle approach** from the list and provide a value for the Tortuosity factor (C).

- Read more about the theory of Non-Newtonian Fluids in Porous Media in the *Polymer Flow Module User's Guide*

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material**. For **User defined** the default value is 1 which is equivalent to free flow.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Depending on the **Flow model** selection in the parent **Porous Medium** feature node you can choose between the following options:

- **Permeability** (the default) to directly enter the permeability of the porous matrix or **Kozeny-Carman** to define the permeability from the porosity and mean **Particle diameter** for **Darcian** flow or
- **Forchheimer** or **Ergun** for **Non-Darcian** flow.

Note that some of these options are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

The default **Permeability** κ(SI unit: m^2) uses the value **From material**, as defined by the **Porous material** list. For **User defined** select **Isotropic** to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value.

For **Kozeny-Carman**, enter the mean **Particle diameter** d_p (SI unit: m), the default value is 0.5 mm.

In case a **Non-Darcian** flow model is chosen in the parent node, **Forchheimer** is the default selection for the **Permeability model**. For **Forchheimer**, the default **Permeability** κ (SI unit: m^2) uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow Module User's Guide*.

- About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*
- Permeability Models in the *Porous Media Flow Module User's Guide*

Mass Source

Enter a value or expression for an optional mass source (or sink) **Source term** Q_m (SI unit: $kg/(m^3 \cdot s)$). This term accounts for mass deposit or mass creation within porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

Effective Mass Transport Parameters

A correction factor (**Bruggeman**, **No Correction**, or **User defined**) to the mass transport parameters (defined in the **Transport Properties** node) can be applied for the porous domain. Species diffusivities and mobilities are automatically adjusted by the porous media corrections. For **User defined** enter a value or expression for the **Conversion factor** f_{eff}. The default is 1. Species diffusivities and mobilities are automatically adjusted by the porous media corrections.

Volume Force

The **Volume Force** node specifies the force $\mathbf{F}$ on the right-hand side of the Navier–Stokes or Brinkman equations, depending on whether a Fluid Properties or Porous Medium node is active on the domain. It then acts on each fluid element in the specified domains.

VOLUME FORCE

Enter the components of the **Volume force** $\mathbf{F}$ (SI unit: N/m^3).

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value. When a turbulence model that solves for the turbulent kinetic energy, k, is used, the option **Include buoyancy-induced turbulence** is available. When selected, the **Buoyancy contribution** is by default set to **Automatic from multiphysics**. Contributions are only obtained from multiphysics couplings that support buoyancy-induced turbulence, such as Nonisothermal Flow. If the **Buoyancy contribution** is switched to **User defined**, a text field for the **Turbulent Schmidt number** appears. See also Theory for Buoyancy-Induced Turbulence in the *CFD Module User's Guide*.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{const}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{const}\mathbf{e_y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

Microfluidic Wall Conditions

Use the **Microfluidic Wall Conditions** node to add boundary conditions to the moving wall and specify whether to use viscous slip or thermal creep.

BOUNDARY CONDITION

The default **Boundary condition** for the wall is **Slip velocity**. Enter values or expressions for the components of the **Velocity of moving wall** $\mathbf{u}_w$ (SI unit: m/s).

Use Viscous Slip

Select the **Use viscous slip** checkbox to define the slip length:

- The default is **User defined**. Enter a value for L_s (SI unit: m). The default is 1e-7 m.
- Select **Maxwell's model** to calculate it from:

$$L_s = \left(\frac{2-\alpha_v}{\alpha_v}\right)\lambda$$

- Then enter values or expressions for the **Tangential momentum accommodation coefficient** (TMAC) α_v (dimensionless) (the default is 0.9) and the **Mean free path** λ (SI unit: m) (the default is 1e-6 m).

Use Thermal Creep

Select the **Use thermal creep** checkbox to activate the thermal creep component of the boundary condition. Enter the fluid's **Temperature** T (SI unit: K) and the **Thermal slip coefficient** σ_T. The default temperature is 293.15 K and the default thermal slip coefficient is 0.75.

If you also have a license for the MEMS Module, an additional **Boundary condition** option **Electroosmotic velocity** is available. This is described in the *MEMS Module User's Guide*.

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls.

BOUNDARY CONDITION

Select a **Boundary condition** for the wall.

- No Slip[1]
- Slip
- Leaking Wall

No Slip

No slip is the default boundary condition for a stationary solid wall for laminar flow (and SST, Low Re k-ε, Algebraic yPlus, L-VEL, and Spalart–Allmaras turbulence models). The condition prescribes $\mathbf{u} = 0$; that is, the fluid at the wall is not moving.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u}\cdot\mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Leaking Wall

This boundary condition can be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_l$ through a perforated wall. The components of the **Fluid velocity** $\mathbf{u}_l$ on the leaking wall should be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( ) and selecting **Advanced Physics Options**.

- Theory for the Wall Boundary Condition
- The Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

The Free and Porous Media Flow, Darcy Interface

The **Free and Porous Media Flow, Darcy** interface ( ) combines the **Darcy's Law** and **Laminar Flow** interfaces to compute fluid velocity and pressure fields where free flow is connected to porous media. The physics interface is suited for situations when both the free flow and the flow in the porous media are laminar.

When a predefined **Free and Porous Media Flow, Darcy** interface is added from the **Porous Media and Subsurface Flow** branch ( ) of the **Model Wizard** or **Add Physics** window, the **Darcy's Law** and **Laminar Flow** interfaces are added to the Model Builder. In addition, the **Multiphysics** node is added, which automatically includes the **Free and Porous Media Flow Coupling** multiphysics coupling.

On the Constituent Physics Interfaces

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows in media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

The **Laminar Flow** interface is used to compute the velocity and pressure for a fluid flow in the laminar flow regime. A flow will remain laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Free and Porous Media Flow, Darcy**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

Free and Porous Media Flow Coupling (Multiphysics Coupling)

The **Free and Porous Media Flow Coupling** multiphysics coupling node ( ) bidirectionally links the **Laminar Flow** and **Darcy's Law** interfaces.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `nsd1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the multiphase flow coupling, or select **All domains** as needed.

When the **Free and Porous Media Flow Coupling** is added as an effect of adding a Free and Porous Media Flow, Darcy multiphysics interface, the selection is the intersection of the boundaries of the participating physics interfaces.

Only boundaries that are active in the participating physics interfaces (which are chosen from the **Coupled Interfaces** selection list) can be selected.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Free flow** and **Porous media flow** lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Free and Porous Media Flow Coupling node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Darcy's Law** is deleted, then the **Porous media flow** list defaults to **None** as there is nothing to couple to.

COUPLING SETTINGS

This section defines the settings for the **Free flow boundary condition**.

- When **No slip** is selected, the tangential component of the fluid velocity at the free-porous interface on the free-flow side (computed in the **Free flow** interface) is set to zero.
- When **Continuous tangential velocity** is selected, the tangential velocity component of the flow on both sides of the free-porous interface is continuous. In addition, continuity of normal stresses and conservation of mass across the interface are ensured.
- When **Beavers-Joseph** is selected, the difference of the tangential velocity components of the flow on both sides of the free-porous interface is proportional to the shear stress at the free-porous interface on the free-flow side. For this option, enter a value or expression for the **Beavers and Joseph parameter** a_{BJ} (dimensionless) that determines the proportionality. In addition, select the checkbox **Use projected permeability** to use only the component of the permeability tensor in the direction of the difference of the tangential velocities on both sides of the interface, instead of the trace of the permeability tensor, in determining the proportionality.
- When **Beavers-Joseph-Saffman** is selected, the tangential velocity component of the flow at the free-porous interface on the free-flow side is proportional to the shear stress at the interface on the free-flow side. For this option also, enter a value or expression for the **Beavers and Joseph parameter** a_{BJ} (dimensionless) that determines the proportionality. In addition, select the checkbox **Use projected permeability** to use only the component of the permeability tensor in the direction of the difference of the tangential velocities on both sides of the interface, instead of the trace of the permeability tensor, in determining the proportionality.
- When **Viscous slip** is selected, the difference of the tangential velocity components of the flow on the free-flow side and a user-supplied interfacial velocity is proportional to the shear stress at the free-porous interface on the free-flow side. Enter values for the **Slip length** L_s (SI unit: m, the default is 1e-7 m), and an **Interfacial velocity** $\mathbf{u}_\mathrm{b}$ (SI unit: m/s, the default is 0 m/s).

In all the above cases, additionally continuity of normal stresses and conservation of mass across the interface are ensured.

Please find related information in the *CFD Module User's Guide*:

- The Darcy's Law Interface
- Theory for the Darcy's Law Interface
- The Laminar Flow Interface
- Theory for the Single-Phase Flow Interfaces
- Theory for the Free and Porous Media Flow, Darcy Interface

The Two-Phase Darcy's Law Interface

The **Two-Phase Darcy's Law (tpdl)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It solves Darcy's law for the total pressure and the transport of the fluid content for one fluid phase. The physics interface can be used to model low velocity flows or media where the permeability and porosity are very small, for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. The physics interface can be used for stationary and time-dependent analyses.

The main feature is the Fluids and Matrix Properties node, which provides an interface for defining the two immiscible fluids properties along with the porous medium properties. The physics interface is available in 2D, 2D axisymmetric, and 3D.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluids and Matrix Properties**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Two-Phase Darcy's Law** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tpdl`.

PHYSICAL MODEL

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is `1[atm]`.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Pressure** and **Fluid content 1**. The name can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION

To display this section, click the **Show More Options** button ( ) and select **Stabilization** from the **Show More Options** dialog.

There are two consistent stabilization methods available — **Streamline diffusion** and **Crosswind diffusion**. **Streamline diffusion** is active by default. The **Residual** setting applies to both the consistent stabilization methods. **Approximate residual** is the default setting and it means that derivatives of the capillary diffusion tensor components are neglected. This setting is usually accurate enough and computationally faster. If required, select **Full residual** instead.

DISCRETIZATION

You can choose the order of the shape functions used for the pressure and fluid content variables solved by the Two-Phase Darcy's Law interface. The default shape functions are **P2+P1** Lagrange.

To display all settings available in this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** from the **Show More Options** dialog.

- Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface
- Theory for the Two-Phase Darcy's Law Interface

Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law Interface has these domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid and Matrix Properties
- Inlet
- Initial Values
- Symmetry
- Interior Wall
- Mass Flux
- No Flux
- Outlet
- Pressure and Saturation

For axisymmetric models, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Fluid and Matrix Properties

The **Fluids and Matrix Properties** node adds Equation 7-20 and Equation 7-21 and defines properties including density, dynamic viscosity, relative permeability, and porosity.

$$\frac{\partial}{\partial t}(\rho\varepsilon_p) + \nabla \cdot (\rho\mathbf{u}) = 0 \tag{7-20}$$

$$\frac{\partial}{\partial t}(c_1\varepsilon_p) + \nabla \cdot (c_1\mathbf{u}) = \nabla \cdot D_c\nabla c_1 \tag{7-21}$$

CAPILLARY MODEL

The list defaults to **Capillary diffusion** or choose **Capillary pressure**.

For **Capillary diffusion**, choose **Isotropic** to define a scalar or **Diagonal**, **Symmetric**, or **Full** to enter a tensor, and then enter values or expressions in the D_c (SI unit: m^2/s) field or fields.

For **Capillary pressure**, select a **Pressure model** — **van Genuchten** (the default), **Brooks and Corey**, or **User defined**.

- For **van Genuchten**, enter an **Entry capillary pressure** p_{ec} (SI unit: Pa), the **Constitutive relations constant** m_{vG} (dimensionless), and **Constitutive relations constant** I_{vG} (dimensionless).
- For **Brooks and Corey**, enter an **Entry capillary pressure** p_{ec} (SI unit: Pa) and the **Pore size distribution index** λ_p (dimensionless).
- For **User defined**, enter a **Capillary pressure** p_c (SI unit: Pa).

FLUID 1 PROPERTIES

Select the material to use for **Fluid 1**. Select **Domain material** (the default value) to use the material defined for the domain. Select another material to use that material's properties.

Define the properties for **Fluid 1**:

The default **Density** ρ_1 (SI unit: kg/m^3) uses values **From material** based on the **Fluid 1** selection. For **User defined** enter another value or expression. The default is 0 kg/m^3.

Select a **Dynamic viscosity** μ_1 (SI unit: Pa·s). The default uses values **From material** as defined by the **Fluid 1** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

Select the **Relative permeability** κ_{r1} (a dimensionless number between 0 and 1) for fluid 1. The default is 1.

FLUID 2 PROPERTIES

The settings to define the properties for **Fluid 2** are similar to those for **Fluid 1**.

MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** (the default) from the **Porous material** list to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From material**, defined by the **Porous material** selection. For **User defined** enter another value or expression The default is 0.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material** selection. For **User defined** select **Isotropic** to define a scalar or **Diagonal**, **Symmetric**, or **Full** to enter a tensor and enter other values or expressions in the field or matrix.

Initial Values

The **Initial Values** node adds initial values for the pressure and the saturation of fluid 1 (that is, the fraction of that fluid inside the pore space) that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa. Enter a value or expression for the initial value of the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1). The default value is 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

No Flux

The **No Flux** node is the default boundary condition stating that there is no flow across impervious boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \mathbf{u} = 0$$

where $\mathbf{n}$ is the vector normal to the boundary.

Also, the No Flux boundary enforces a zero gradient condition for the fluid content across the selected boundary

$$\mathbf{n} \cdot \nabla c_1 = 0$$

Pressure and Saturation

Use the **Pressure and Saturation** node to specify the pressure and fluid volume fractions on a boundary. In many cases the distribution of pressure and saturation are known as numbers, distributions, or expressions involving time, t, for example.

PRESSURE AND SATURATION

Enter a value or expression for the **Pressure** p (SI unit: Pa), and for the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1). The default values are 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

Mass Flux

Use the **Mass Flux** node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain

$$-\mathbf{n} \cdot \rho \mathbf{u} = N_0$$

where N_0 is a value or expression for the inward (or outward) Darcy's flux that is specified.

MASS FLUX AND SATURATION

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: kg/(m^2·s)). A positive value of N_0 represents an inward mass flux, whereas a negative value represents an outward mass flux.

Enter a value or expression for the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1) in the mass flux. The default value is 0.

Inlet

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot \rho\mathbf{u} = (s_1\rho_1 + s_2\rho_1)U_0$$

where U_0 is a specified value or expression for the inward (or outward) Darcy's velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas a negative value represents an outflow.

INLET

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity, whereas a negative value represents an outward velocity.

Enter a value or expression for the **Saturation fluid 1** s_1 (a dimensionless number between 0 and 1). The default value is 0.

Outlet

The **Outlet** node adds a boundary condition for the outflow perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot D_c\nabla c_1 = 0$$

where D_c is the capillary diffusion (SI unit: m^2/s) and $c_1 = s_1\rho_1$ is the fluid 1 content (SI unit: kg/m^3). This means that the normal gradient of fluid saturation does not change through this boundary.

PRESSURE

Enter a value or expression for the **Pressure** p. The default value is 0. If the reference pressure p_{ref}, defined at the physics interface level is 0, enter the absolute pressure. Otherwise, enter the relative pressure.

Symmetry

The **Symmetry** node describes a symmetry boundary where there is no tangential flow. The following condition implements the symmetry condition on an axis or a flow divide:

$$-\mathbf{n} \cdot \rho \mathbf{u} = 0$$

$$-\mathbf{n} \cdot D_c \nabla c_1 = 0$$

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries.

It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an internal boundary. It allows discontinuities of velocity and pressure across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

Thin Barrier

The **Thin Barrier** boundary condition can only be applied on interior boundaries.

It is similar to the **Interior Wall** boundary available on interior boundaries except that it allows pressure and concentration gradients across the boundary. The **Thin Barrier** boundary condition can be used to avoid meshing thin permeable structures by applying flux condition on interior curves and surfaces instead.

The Multiphase Flow in Porous Media Interface

The **Multiphase Flow in Porous Media** interface ( ) combines the **Darcy's Law** interface with the **Phase Transport in Porous Media** interface to model the flow and transport of multiple immiscible phases in a porous medium.

When a predefined **Multiphase Flow in Porous Media** interface is added from the **Porous Media and Subsurface Flow** branch ( ) of the **Model Wizard** or **Add Physics** window, **Phase Transport** and **Darcy's Law** interfaces are added to the Model Builder. In addition, the **Multiphysics** node is added, which automatically includes the **Multiphase Flow in Porous Media** multiphysics coupling.

On the Constituent Physics Interfaces

The **Phase Transport in Porous Media** interface is used to simulate the transport of immiscible multiple species in a porous medium and solves for their averaged volume fractions (also called saturations). The interfaces between the different phases are not tracked explicitly, although microscopic interfacial effects are taken into account in the macroscopic equations through the capillary pressure functions.

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows in media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Multiphase Flow in Porous Media**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Phase Transport in Porous Media** and **Darcy's Law** interfaces are added, an empty **Multiphysics** node appears in the model tree. You can choose from the

available coupling features but the settings in the constituent interfaces are not modified.

TABLE 7-2: MODIFIED SETTINGS FOR A MULTIPHASE FLOW IN POROUS MEDIA INTERFACE.

PHYSICS INTERFACE OR COUPLING FEATURE	MODIFIED SETTINGS
Darcy's Law	In the Darcy's Law interface, linear shape functions are used for the discretization of the pressure.
Multiphase Flow in Porous Media	The **Domain Selection** is the same as that of the participating physics interfaces. The corresponding Phase Transport in Porous Media and Darcy's Law interfaces are preselected in the Coupled Interfaces section.

Multiphase Flow in Porous Media (Multiphysics Coupling)

The **Multiphase Flow in Porous Media** multiphysics coupling node ( ) links bidirectionally the **Phase Transport in Porous Media** and **Darcy's Law** interfaces.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `mfpm1`.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the multiphase flow coupling, or select **All domains** as needed.

When **Multiphase Flow in Porous Media** is added as an effect of adding a Multiphase Flow in Porous Media interface, the selection is the same as for the participating physics interfaces.

Only domains that are active in the participating physics interfaces (which are chosen from the **Coupled Interfaces** selection list) can be selected.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Phase transport** and **Flow in porous media** lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Multiphase Flow in Porous Media node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Darcy's Law** is deleted, then the **Flow in porous media** list defaults to **None** as there is nothing to couple to.

Please find related information under

- The Phase Transport Interfaces and
- Theory for the Phase Transport Interfaces

in the *CFD Module User's Guide*.

Well (Multiphysics Coupling)

The **Multiphase Flow in Porous Media** ( ) interface contains an optional **Well** multiphysics coupling feature on points (in 2D) or edges (in 3D). The **Well** coupling node is intended to model injection or production wells and links bidirectionally the **Phase Transport in Porous Media** and **Darcy's Law** interfaces.

The Subsurface Flow Module license is required to use this coupling feature (see https://www.comsol.com/products/specifications/).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Well** multiphysics coupling feature in the model) is `wellmpp1`.

POINT OR EDGE SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific points or edges, or select **All points** or **All edges** as needed.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Phase transport** or **Flow in porous media** lists

WELL

Select whether the well is a production or injection well: for an injection well positive mass fluxes signify inflowing fluxes and for a production well positive mass fluxes are outflowing fluxes.

Either specify the total **Total mass flow rate** M_0 (SI unit: kg/s), the **Total mass flow rate per unit length** M_l (SI unit: kg/(m·s)), the **Pressure** p_0 (SI unit: Pa), the **Pressure head** H_p0 (SI unit: m), or the **Hydraulic head** H_0 (SI unit: m). The elevation D used to convert the hydraulic head to a pressure, is defined by the gravity effects in the coupled Darcy's Law interface.

Select the **Specify well diameter** checkbox to define the **Well diameter** d_w (SI unit: m). This averages the mass source on the boundary of a cylinder around the line. This option avoids obtaining an increasing pressure value at the line when meshing finer than this diameter. It makes use of the `circavg` operator.

If the well diameter is defined, the option to specify the **Total mass flux** N_0 (SI unit: kg/(m^2·s)) is also available.

PHASES

The number of **Phase** sections depends on the number of phases defined in the coupled Phase Transport in Porous Media interface: the number of sections is equal to the number of phases not computed from the volume constraint, which is in turn equal to the number of phases defined in the coupled Phase Transport in Porous Media interface minus one.

Specify the boundary condition for each phase not computed from the volume constraint. You can choose to enter a value for the **Mass flow rate** $M_{0,i}$ (SI unit: kg/s), the **Mass flow rate per unit length** $M_{\mathrm{l},i}$ (SI unit: kg/(m·s)), or the **Volume fraction** $s_{0,i}$ (dimensionless). If the well diameter is specified, the option to specify the **Mass flux** $N_{0,i}$

(SI unit: kg/(m^2·s)) is also available. For a production well, you can additionally choose the **Outflow** option. For an injection well you can additionally choose to specify the **Fraction of total volumetric flow rate** $s_{0,i}$ (dimensionless).

Fraction of total volumetric flow rate

When the **Fraction of total volumetric flow rate** $s_{0,i}$ is specified for a phase, a mass flow rate per unit length $M_{1,i}$ is supplied for that phase, which is given by

$$M_{1,i} = \rho_i s_{0,i} V_1 \tag{7-22}$$

where V_1 is the total volumetric flow rate per unit length, which is computed as follows: assume that there are N phases, and that phase 1 is the phase computed from the volume constraint, that for phases i, for $i = 2, ..., p$, the fraction of total volumetric flow rate $s_{0,i}$ is supplied, and that for the phases i, for $i = p+1, ..., N$, the mass flow rate per unit length $M_{1,i}$ is given. Then V_1 can be computed from the relation

$$V_1 = \frac{M_{1,1}}{\rho_1} + \sum_{i=2}^{p} V_1 s_{i,0} + \sum_{i=p+1}^{N} \frac{M_{1,i}}{\rho_i} \tag{7-23}$$

where the mass flow rate $M_{1,1}$ for the phase computed from the volume constraint is given by

$$M_{1,1} = M_1 - \sum_{i=2}^{p} V_1 \rho_i s_{i,0} - \sum_{i=p+1}^{N} M_{1,i} \tag{7-24}$$

Note that the total mass flow rate per unit length M_1 is readily available when any of the **Total mass flow rate**, **Total mass flow rate per unit length**, or the **Total mass flux** options is chosen. Furthermore, the total mass flow rate per unit length M_1 is also available as a Lagrange multiplier in case any of the **Pressure**, the **Pressure head**, or the **Hydraulic head** is given, as these conditions are implemented as weak constraints. For the mass flow rates per unit length $M_{1,i}$ of the individual phases, it holds similarly that they are readily available when any of the **Mass flow rate**, **Mass flow rate per unit length**, or the **Mass flux** options are chosen, and that for the **Volume fraction** option, implemented as a weak constraint, the mass flow rate per unit length $M_{1,i}$ is computed as a Lagrange multiplier.

Outflow

When the **Outflow** option is specified for a phase s_i, an outflowing mass flow rate per unit length $M_{1,i}$ is supplied for that phase, which is given by

$$M_{\mathrm{l},i} = \frac{\rho_i \kappa_{\mathrm{r}i}}{\lambda_{\mathrm{r}} \mu_i} M_{\mathrm{l}} \qquad \text{with} \quad \lambda_{\mathrm{r}} = \sum_{i=1}^{N} \frac{\rho_i \kappa_{\mathrm{r}i}}{\mu_i} \tag{7-25}$$

where $\kappa_{\mathrm{r}i}$ denotes the relative permeability of phase i.

Thin Barrier (Multiphysics Coupling)

The **Multiphase Flow in Porous Media** ( ) interface contains an optional **Thin Barrier** multiphysics coupling feature on edges (in 2D) or surfaces (in 3D). The **Thin Barrier** coupling node can be used to avoid meshing interior permeable structures that are less permeable than the adjacent porous domains. It links bidirectionally the **Phase Transport in Porous Media** and **Darcy's Law** interfaces.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Thin Barrier** multiphysics coupling feature in the model) is `tbls1`.

BOUNDARY SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific boundaries, or select **All boundaries** as needed.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Phase transport** or **Flow in porous media** lists

SHELL PROPERTIES

The **Thin Barrier** multiphysics coupling feature is designed to be only applicable for a **Single Layer Material**. Select the **Single Layer Material** to be used for the thin barrier from the **Layer** list. The **Thickness** of the thin barrier is set in the **Layer Definition** section of the **Shell Property Group** window of the **Single Layer Material**. Also use this section to set the number of **Mesh elements** that are used in the Extra Dimension to solve the equations through the thickness of the thin barrier layer.

MODEL INPUT

The material properties of the different phases, such as density and viscosity, can be defined through user inputs, variables, or by selecting a boundary material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties. These model inputs appear in this section.

MATRIX PROPERTIES

Select the material to use as porous matrix inside the thin barrier. Select **Boundary material** (the default) from the **Porous material** list to use the material defined for the thin barrier boundary. Select another material to use that material's properties.

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From material**, defined by the **Porous material** selected. For **User defined** the default is 0.5.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the **Porous material** selected. For **User defined** the default is `1e-9` m^2.

CAPILLARY PRESSURE

Select a **Capillary pressure model** — **User defined** (the default), **van Genuchten**, **Brooks and Corey**, or **Capillary diffusion**. The **van Genuchten** and **Brooks and Corey** options are only available when there are not more than two phases present in the model.

- For **User defined**, enter an expression for the **Capillary pressure** p_c (SI unit: Pa) for the phases that are not computed from the volume constraint. The pressure of the corresponding phase is equal to the pressure of the phase computed from the volume constraint plus the capillary pressure supplied for this phase.
- For **van Genuchten**, enter an **Entry capillary pressure** p_{ec} (SI unit: Pa), the **Constitutive relations constant** m_{vG} (dimensionless), and **Constitutive relations constant** l_{vG} (dimensionless).
- For **Brooks and Corey**, enter an **Entry capillary pressure** p_{ec} (SI unit: Pa) and the **Pore size distribution index** λ_p (dimensionless).
- For **Capillary diffusion**, enter a capillary diffusion coefficient D_c (SI unit: m^2/s) for the phases that are not computed from the volume constraint.

PHASE PROPERTIES

Select the material to use for each phase. Select **Boundary material** (the default) from the **Fluid** list to use the material defined for the domain. Select another material to use that material's properties.

Enter the **Density** ρ (SI unit: kg/m^3), **Dynamic viscosity** μ (SI unit: Pa·s) and **Relative permeability** κ_r (a dimensionless number between 0 and 1) for each phase. The defaults for the **Density** and **Dynamic viscosity** are **From material**, and **User defined** for the **Relative permeability**. For **User defined**, the default values are 1000 kg/m^3, 0.001 Pa·s. and s_i^2, respectively.

The **Relative permeability** input fields are only available when the **Capillary pressure model** is set to **User defined** or **Capillary diffusion**. In the other cases (**van Genuchten** or **Brooks and Corey**) the relative permeabilities are defined by the **van Genuchten** or **Brooks and Corey** model. For the **van Genuchten** and **Brooks and Corey** model, specify the **Residual saturation** s_{ri} (dimensionless, default value 0) for each phase.

INITIAL VALUES

Enter a value or expression in the field for the volume fraction inside the thin barrier of each phase, except for the one computed from the volume constraint, and in the field for the pressure of the phase computed from the volume constraint.

Please find related information under

- Single Layer Materials in the *COMSOL Multiphysics Reference Manual* and
- Theory for the Multiphase Flow in Porous Media Interface in the *Subsurface Flow Module User's Guide*.

The Multiphase Free and Porous Media Flow Interface

The **Multiphase Free and Porous Media Flow** interface ( ) combines the **Phase Transport in Free and Porous Media** interface with the **Darcy's Law** and **Laminar Flow** interfaces to model the transport of multiple immiscible phases in coupled free and porous media flow.

When a predefined **Multiphase Free and Porous Media Flow** interface is added from the **Porous Media and Subsurface Flow** branch ( ) of the **Model Wizard** or **Add Physics** window, the **Phase Transport in Free and Porous Media, Darcy's Law** and **Laminar Flow** interfaces are added to the Model Builder. In addition, the **Multiphysics** node is added, which automatically includes the **Multiphase Flow in Porous Media**, the **Mixture Model**, and the **Free and Porous Media Flow Coupling** multiphysics couplings.

On the Constituent Physics Interfaces

The **Phase Transport in Free and Porous Media Flow** interface is used to simulate the transport of multiple immiscible species in free and porous media flow and solves for their averaged volume fractions (also called saturations). The interfaces between the different phases are not tracked explicitly, although microscopic interfacial effects are taken into account in the macroscopic equations through the capillary pressure functions in porous domains.

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows in media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

The **Laminar Flow** interface is used to compute the velocity and pressure for a fluid flow in the laminar flow regime. A flow will remain laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Multiphase Free and Porous Media Flow**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

TABLE 7-3: MODIFIED SETTINGS FOR A MULTIPHASE FREE AND POROUS MEDIA FLOW INTERFACE.

PHYSICS INTERFACE OR COUPLING FEATURE	MODIFIED SETTINGS
Darcy's Law	In the Darcy's Law interface, linear shape functions are used for the discretization of the pressure.
Multiphase Flow in Porous Media	The **Domain Selection** is the same as that of the participating physics interfaces. The corresponding Phase Transport in Free and Porous Media Flow and Darcy's Law interfaces are preselected in the Coupled Interfaces section.
Mixture Model	The **Domain Selection** is the same as that of the participating physics interfaces. The corresponding Phase Transport in Free and Porous Media Flow and Laminar Flow interfaces are preselected in the Coupled Interfaces section.
Free and Porous Media Flow Coupling	The **Boundary Selection** is the same as that of the participating physics interfaces. The corresponding Laminar Flow and Darcy's Law interfaces are preselected in the Coupled Interfaces section.

Coupling Features

Three coupling features are added: The Multiphase Flow in Porous Media (Multiphysics Coupling), the Free and Porous Media Flow Coupling (Multiphysics Coupling), and the Mixture Model multiphysics coupling.

Please find related information under

- Theory for the Phase Transport Mixture Model Interfaces
- Theory for the Free and Porous Media Flow, Darcy Interface
- Theory for the Multiphase Flow in Porous Media Interface

in the *CFD Module User's Guide*.

The Thin-Film and Porous Media Flow Interface

The **Thin-Film and Porous Media Flow** interface ( ) combines the **Thin-Film Flow** interface with the **Darcy's Law** interface. It couples the flow of a thin film of fluid in a channel, represented by a boundary in the geometry, with a low velocity fluid flow in a porous medium, represented by a domain in the geometry.

When a predefined **Thin-Film and Porous Media Flow** interface is added from **Porous Media and Subsurface Flow** branch ( ) of the **Model Wizard** or **Add Physics** window, **Thin-Film Flow** and **Darcy's Law** interfaces are added to the Model Builder. In addition, the **Multiphysics** node is added, which automatically includes the **Thin-Film and Porous Media Flow** multiphysics coupling.

On the Constituent Physics Interfaces

The **Thin-Film Flow** interface is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by a boundary within the geometry. It is used for lubrication, elastohydrodynamics, or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the modified Reynolds equation to apply.

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined coupling, for example **Thin-Film and Porous Media Flow**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling feature, these modified settings are not automatically included.

For example, if single **Thin-Film Flow** and **Darcy's Law** interfaces are added, an empty **Multiphysics** node appears in the model tree. You can choose from the available coupling features but the settings in the constituent interfaces are not modified.

Thin-Film and Porous Media Flow (Multiphysics Coupling)

The **Thin-Film and Porous Media Flow** multiphysics coupling node ( ) links bidirectionally the **Thin-Film Flow** and **Darcy's Law** interfaces.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `tfpf1`.

BOUNDARY SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific boundaries to define the multiphase flow coupling, or select **All boundaries** as needed.

When **Thin-Film and Porous Media Flow** multiphysics coupling node is added by the predefined **Thin-Film and Porous Media Flow** interface, the selection is the intersection of selections of boundaries of the participating physics interfaces.

Only boundaries that belong to the participating physics interfaces (which are chosen from the **Coupled Interfaces** selection list) can be selected.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Thin-film flow** and **Porous media flow** lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Multiphase Flow in Porous Media node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Darcy's Law** is deleted, then the **Porous media flow** list defaults to **None** as there is nothing to couple to.

COUPLING

This section defines the options available for the **Coupling type** between the **Thin-film flow** interface and the **Porous media flow** interface.

- Choose **No-slip condition** if the fluid velocity in the **Porous media flow** interface and the fluid velocities at the wall and base of the **Thin-film flow** interface are mutually independent. The coupling does not introduce additional velocity constraints in the **Thin-film flow** interface. However, it ensures the continuity of pressure and accounts for mass flux across the interface.
- Choose **Beavers-Joseph slip condition** if the development of the boundary layer at the intersection of the physics interfaces needs to be modeled using a small interface slip velocity. The coupling introduces constraints on the fluid velocities at the wall and base in the **Thin-film flow** interface which depend on the fluid velocity in the **Porous media flow** interface. Additionally, it ensures the continuity of pressure and accounts for mass flux across the interface. This option is only available when the **Film flow model** selected in the **Fluid Film Properties** of the **Thin-film flow** interface is either **No-slip walls** or **Slip at walls**. Also, specify the Beavers–Joseph slip coefficient at the wall and the base boundaries.

- Theory for the Thin-Film Flow Interfaces
- Theory for the Darcy's Law Interface
- Theory for the Thin-Film and Porous Media Flow Interface

Squeeze Film Between Rectangular Porous and Nonporous Plates: Application Library path **CFD_Module/Verification_Examples/squeeze_film_porous**

Self-Lubricating Journal Bearing: Application Library path **CFD_Module/Verification_Examples/self_lubricating_bearing**

Theory for the Darcy's Law Interface

The Darcy's Law Interface theory is described in this section:

- About Darcy's Law
- Darcy's Law — Equation Formulation
- Storage Models
- Average Linear Velocity
- Dual Porosity and Dual Permeability Theory
- References for the Darcy's Law Interface

About Darcy's Law

In a porous medium, the global transport of momentum by shear stresses in the fluid is often negligible, because the pore walls impede momentum transport to the fluid outside the individual pores. A detailed description, down to the resolution of every pore, is not practical in most applications. A homogenization of the porous and fluid media into a single medium is a common alternative approach. Darcy's law together with the continuity equation and equation of state for the pore fluid (or gas) provide a complete mathematical model suitable for a wide variety of applications involving porous media flows, for which the pressure gradient is the major driving force.

Darcy's law describes fluid movement through interstices in a porous medium. Because the fluid loses considerable energy to frictional resistance within pores, flow velocities in porous media are very low. The Darcy's Law interface can be applied to small-scale tasks in chemical engineering as well as to large-scale geophysical or hydrological tasks such as water moving in an aquifer or stream bank, oil migrating to a well, and even magma rising through the earth to a chamber in a volcano (see Ref. 1, Ref. 2, Ref. 3, and Ref. 4). Also set up multiple Darcy's Law interfaces to model multiphase flows involving more than one mobile phase.

Darcy's law describes flow in porous media driven by gradients in the hydraulic potential field, which has units of pressure. For many applications it is convenient to represent the total hydraulic potential or the pressure and the gravitational components with equivalent heights of fluid or head. Division of potential by the fluid weight can simplify modeling because units of length make it straightforward to compare to many physical data. Consider, for example, fluid levels in wells, stream heights, topography, and velocities. The physics interface also supports specifying

boundary conditions and result evaluation using hydraulic head and pressure head. In the physics interface, pressure is always the dependent variable.

Darcy's Law — Equation Formulation

Darcy's law states that the velocity field is determined by the pressure gradient, the fluid viscosity, and the structure of the porous medium:

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{7-26}$$

In this equation, $\mathbf{u}$ is the Darcy's velocity or specific discharge vector (SI unit: m/s); κ is the permeability of the porous medium (SI unit: m^2); μ is the fluid's dynamic viscosity (SI unit: Pa·s); p is the pore pressure (SI unit: Pa) and ρ is the density of the fluid (SI unit: kg/m^3).

- The above equation formulation is called linear Darcy's law. The applicability of this formulation is discussed in the chapter About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*.
- Permeability can be defined in different ways, either directly or based on predefined permeability models. These are described in detail in the chapter Permeability Models.
- For a detailed overview of the permeability models available in each product visit https://www.comsol.com/products/specifications/.

The Darcy's Law interface combines Darcy's law with the continuity equation

$$\frac{\partial}{\partial t}(\rho\varepsilon_p) + \nabla\cdot(\rho\mathbf{u}) = Q_m \tag{7-27}$$

In the above equation, ρ is the fluid density (SI unit: kg/m^3), ε_p is the porosity, and Q_m is a mass source term (SI unit: $kg/(m^3\cdot s)$). Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

For large-scale applications it might be necessary to take gravity effects into account. Darcy's law then applies when the gradient in hydraulic potential drives fluid movement in the porous medium. Darcy's law then has the form:

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p - \rho \mathbf{g}) \tag{7-28}$$

- See the section Gravity Effects in the *Subsurface Flow Module User's Guide*.
- Note that gravity effects are only included in some modules. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.
- Gravity effects are not active by default. Select the checkbox **Include gravity** to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

Storage Models

The continuity equation (Equation 7-27) allows flexible specification of relationships between parameters like density or permeability with respect to variables such as pressure, temperature, concentration, and more.

Expanding the time-derivative term and defining the porosity and density as functions of the pressure and using the chain rule results in

$$\frac{\partial}{\partial t}(\rho \varepsilon_p) = \varepsilon_p \frac{\partial \rho}{\partial t} + \rho \frac{\partial \varepsilon_p}{\partial t} = \varepsilon_p \frac{\partial \rho}{\partial p}\frac{\partial p}{\partial t} + \rho \frac{\partial \varepsilon_p}{\partial p}\frac{\partial p}{\partial t}$$

By inserting the definition of fluid compressibility $\chi_f = (1/\rho)(\partial\rho/\partial p)$ to the right-hand side and rearrange the following expression is obtained

$$\frac{\partial(\rho \varepsilon_p)}{\partial t} = \rho\left(\varepsilon_p \chi_f + \frac{\partial \varepsilon_p}{\partial p}\right)\frac{\partial p}{\partial t} = \rho S_p \frac{\partial p}{\partial t}$$

Using this relation, the generalized governing equation (Equation 7-27) takes the following form:

$$\rho S_p \frac{\partial p}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{7-29}$$

In this equation, S_p is the storage coefficient (SI unit: 1/Pa), which can be interpreted as the weighted compressibility of the porous material and the fluid. The storage can be an expression involving results from a solid-deformation equation or an expression involving temperatures and concentrations from other analyses. The Darcy's Law

interface implements Equation 7-29 in the **Porous Medium** node, which explicitly includes different storage models to choose from:

- **From density and porosity**, where the storage directly depends on changes in porosity or fluid density
- **Linearized storage**, which defines S_p using the compressibility of the fluid χ_f and of the porous matrix χ_p according to

$$S_p = \varepsilon_p \chi_f + (1 - \varepsilon_p)\chi_p$$

- **Poroelastic storage** where

$$S_p = \varepsilon_p \chi_f .$$

Storage models are only available for the Subsurface Flow Module and the Porous Media Flow Module. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Average Linear Velocity

Because fluids typically occupy only 10% to 50% of a porous medium, it follows that velocities within the pore channels exceed the Darcy velocity, $\mathbf{u}$, on the order of two to ten times. For clarity, the physics interface includes the average linear velocity within the pores, $\mathbf{u}_\alpha$, (also termed the seepage velocity) defined as $\mathbf{u}_\alpha = \mathbf{u}/\varepsilon_p$, where ε_p is the porosity.

Dual Porosity and Dual Permeability Theory

The first well known publication on this topic is "The Behavior of Naturally Fractured Reservoirs" by J.E. Warren and P.J. Root from 1963. Since then the researchers further developed the idea of a dual porosity/permeability type of a porous medium. One of the well established models is based on the findings of H. Gerke and M. van Genuchten (Ref. 9). Basically the idea behind is to solve for each part of the porous medium (macro- and micropores) the relevant equations and connect them via an exchange term.

DUAL POROSITY MEDIUM

Darcy's Law is solved for the macropores and taking into account their volume fraction θ_M the equation reads:

$$\theta_M\left(\rho S_{\mathrm{p,M}}\frac{\partial p_{\mathrm{M}}}{\partial t}+\nabla(\rho\mathbf{u}_{\mathrm{M}})\right) = \theta_{\mathrm{M}}Q_{\mathrm{M}}-Q_{\mathrm{ip}} \tag{7-30}$$

The term Q_{ip} describes the mass source from the Interporosity Flow which is the mass transfer from the macropores to the micropores system. An additional ODE for the (passive) micropores is solved which only act as additional storage volume:

$$(1-\theta_M)\left(\rho S_{\mathrm{p,m}}\frac{\partial p_{\mathrm{m}}}{\partial t}\right) = (1-\theta_{\mathrm{M}})Q_{\mathrm{M}}+Q_{\mathrm{ip}}\,.$$

The indices M and m stand for macropores and micropores, respectively.

DUAL PERMEABILITY MEDIUM

Darcy's law has to be solved for both the macroscale system and the microscale system:

$$\begin{gathered}\theta_{\mathrm{M}}\left(\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p,M}}\rho)+\nabla\cdot(\rho\mathbf{u}_{\mathrm{M}})\right) = -Q_{\mathrm{ip}}+\theta_{\mathrm{M}}Q_{\mathrm{m}}\\ (1-\theta_{\mathrm{M}})\left(\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p,m}}\rho)+\nabla\cdot(\rho\mathbf{u}_{\mathrm{m}})\right) = Q_{\mathrm{ip}}+(1-\theta_{\mathrm{M}})Q_{\mathrm{m}}\\ p = \theta_{\mathrm{M}}p_{\mathrm{M}}+(1-\theta_{\mathrm{M}})p_{\mathrm{m}}\end{gathered} \tag{7-31}$$

θ_{M} is the volume fraction of the macropores, Q_{ip} denotes the interporosity flow, signifying the mass transfer from the macropores (identified by index M) to the micropores (identified by index m).

Solving Darcy's law for both systems entails solving two equations, each associated with dependent pressure variables p_{m} and p_{M}. These equations are coupled via Q_{ip}. From this, average quantities for the dual permeability medium as a whole are computed. The average pressure of the dual permeability medium is defined as:

$$p = \theta_{\mathrm{M}}p_{\mathrm{M}}+(1-\theta_{\mathrm{M}})p_m$$

Likewise, average values for permeability, storage, velocity and other relevant parameters are computed.

UNSATURATED DUAL PERMEABILITY MEDIUM

Use the **Unsaturated Dual Permeability Medium** feature to model the transport in an unsaturated dual permeability medium where Richards' Equation (Equation 4-26) describes the transport in each system.

$$\theta_M\left(\rho\left(S_{e,M}S_{p,M}+\frac{C_{m,M}}{\rho g}\right)\frac{\partial p_M}{\partial t}+\nabla(\rho\mathbf{u}_M)\right)=-Q_{ip}+\theta_M Q_m$$
$$(1-\theta_M)\left(\rho\left(S_{e,m}S_{p,m}+\frac{C_{m,m}}{\rho g}\right)\frac{\partial p_m}{\partial t}+\nabla(\rho\mathbf{u}_m)\right)=Q_{ip}+(1-\theta_M)Q_m \quad (7\text{-}32)$$
$$p=\theta_M p_M+(1-\theta_M)p_m$$

θ_M is the volume fraction of the macropores, Q_{ip} is the interporosity flow which is the mass transfer from the macroscale to the microscale system. The indices **M** and **m** stand for macropores and micropores, respectively.

INTERPOROSITY FLOW

Specify the **Fluid Transfer Function** α_w which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{ip}=\alpha_w(p_M-p_m) \quad (7\text{-}33)$$

with p_M being the pressure within the macroscale system and p_m the pressure within the microscale system

References for the Darcy's Law Interface

1. J. Bear, *Hydraulics of Groundwater*, McGraw Hill, 1979.

2. S.E. Ingebritsen and W.E. Sanford, *Groundwater in Geologic Processes*, Cambridge University Press, 1998.

3. N.H. Sleep and K. Fujita, *Principles of Geophysics*, Blackwell Science, 1997.

4. D.L. Turcotte and G. Schubert, *Geodynamics*, Cambridge University Press, 2002.

5. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing, 1972.

6. Ö. Akgiray and A.M. Saatçı, "A New Look at Filter Backwash Hydraulics," *Water Sci. Technol. Water Supply*, vol. 1, no. 2, pp. 65–72, 2001.

7. L. Klinkenberg, "The permeability of porous media to liquids and gases," *Drilling and Production Practice*, Am. Petroleum Inst., pp. 200–213, 1941.

8. Yu-Shu Wu and others, "Gas Flow in Porous Media with Klinkenberg Effects," *Transp. Porous Media*, vol. 32, pp. 117–137, 1998.

9. H. Gerke and M. van Genuchten, "A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media," *Water Resour. Res.*, vol. 29. pp. 305–319. 1993.

Theory for the Brinkman Equations Interface

The Brinkman Equations Interface theory is described in this section:

- About the Brinkman Equations
- Brinkman Equations Theory
- References for the Brinkman Equations Interface

About the Brinkman Equations

The ***Brinkman equations*** describe fluids in porous media for which the momentum transport within the fluid due to shear stresses is of importance. This mathematical model extends Darcy's law to include a term that accounts for the viscous transport in the momentum balance, and it treats both the pressure and the flow velocity vector as independent variables. Use the Free and Porous Media Flow, Brinkman interface to model combinations of porous media and free flow domains. These types of problems are often encountered in applications such as monolithic reactors and fuel cells.

The Free and Porous Media Flow, Brinkman Interface

In porous domains, the flow variables and fluid properties are defined at any point inside the medium by means of averaging of the actual variables and properties over a certain volume surrounding the point. This control volume must be small compared to the typical macroscopic dimensions of the problem, but it must be large enough to contain many pores and solid matrix elements.

Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

The physical properties of the fluid, such as density and viscosity, are defined as *intrinsic volume averages* that correspond to a unit volume of the pores. Defined this way, they present the relevant physical parameters that can be measured experimentally, and they are assumed to be continuous with the corresponding parameters in the adjacent free flow.

The flow velocity is defined as a *superficial volume average*, and it corresponds to a unit volume of the medium including both the pores and the matrix. It is sometimes called the Darcy velocity, defined as the volume flow rate per unit cross section of the medium. Such a definition makes the velocity field continuous across the boundaries between porous regions and regions of free flow.

Brinkman Equations Theory

The dependent variables in the Brinkman equations are the Darcy velocity and the pressure. The flow in porous media is governed by a combination of the continuity equation and the momentum equation, which together form the Brinkman equations:

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_m \tag{7-34}$$

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) = -\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_m}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F} \tag{7-35}$$

In these equations:

- μ (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- $\mathbf{u}$ (SI unit: m/s) is the velocity vector
- ρ (SI unit: kg/m^3) is the density of the fluid
- p (SI unit: Pa) is the pressure
- ε_p is the porosity
- κ (SI unit: m^2) is the permeability of the porous medium, and
- Q_m (SI unit: kg/(m^3·s)) is a mass source or sink

Influence of gravity and other volume forces can be accounted for via the force term $\mathbf{F}$ (SI unit: kg/(m^2·s^2)).

When the **Neglect inertial term (Stokes flow)** checkbox is selected, the term $(\mathbf{u} \cdot \nabla)(\mathbf{u}/\varepsilon_p)$ on the left-hand side of Equation 7-19 is disabled.

The mass source, Q_m, accounts for mass deposit and mass creation within the domains. The mass exchange is assumed to occur at zero velocity.

The Forchheimer and Ergun drag options add a viscous force proportional to the square of the fluid velocity, $\mathbf{F} = -\rho\beta|\mathbf{u}|\mathbf{u}$, on the right-hand side of Equation 7-19; see References for the Darcy's Law Interface for details.

In case of a flow with variable density, Equation 7-18 and Equation 7-19 must be solved together with the equation of state that relates the density to the temperature and pressure (for instance the ideal gas law).

For incompressible flow, the density stays constant in any fluid particle, which can be expressed as

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \mathbf{u} \cdot \nabla \rho = 0$$

and the continuity equation (Equation 7-18) reduces to

$$\rho \nabla \cdot \mathbf{u} = Q_m$$

References for the Brinkman Equations Interface

1. D. Nield and A. Bejan, *Convection in Porous Media*, 3rd ed., Springer, 2006.

2. M. Le Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

Theory for the Free and Porous Media Flow, Brinkman Interface

The Free and Porous Media Flow, Brinkman Interface uses the Navier–Stokes equations to describe the flow in open regions, and the Brinkman equations to describe the flow in porous regions.

The same fields, $\mathbf{u}$ and p, are solved for in both the free flow domains and in the porous domains. This means that the pressure in the free fluid and the pressure in the pores is continuous over the interface between a free flow domain and a porous domain. It also means that continuity is enforced between the fluid velocity in the free flow and the Darcy velocity in the porous domain. This treatment is one of several possible models for the physics at the interface. Examples of other models can be found in Ref. 1.

The continuity in $\mathbf{u}$ and p implies a stress discontinuity at the interface between a free-flow domain and a porous domain. The difference corresponds to the stress absorbed by the rigid porous matrix, which is a consequence implicit in the formulations of the Navier–Stokes and Brinkman equations.

Reference for the Free and Porous Media Flow, Brinkman Interface

1. M.L. Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

Theory for the Free and Porous Media Flow, Darcy Interface

The **Free and Porous Media Flow, Darcy** interface uses the Navier–Stokes equations to describe the flow in the free-flow region, implemented by the coupled Laminar Flow interface, and Darcy's law, implemented by the coupled Darcy's Law interface, to describe the flow in the porous region.

In the free-flow region, the velocity u and pressure p are solved for, whereas in the porous region only the pressure p is solved for, and the velocity is calculated from the pressure by Darcy's law.

The coupling between the free and porous medium flow, implemented by the Free and Porous Media Flow Coupling, ensures conservation of mass across the free-porous interface, which is enforced by the condition

$$\mathbf{n} \cdot (\rho_{ns}\mathbf{u}_{ns}) = \mathbf{n} \cdot (\rho_{d}\mathbf{u}_{d}) \tag{7-36}$$

Here ρ_{ns} and $\mathbf{u}_{ns}$ are the density and velocity on the free-flow side of the interface, ρ_{d} and $\mathbf{u}_{d}$ the density and velocity on the porous side, and $\mathbf{n}$ is a vector normal to the interface. In addition the coupling enforces the balance of the normal forces by:

$$p_{ns} - \mathbf{n} \cdot \mathbf{K}\mathbf{n} = p_{d} \tag{7-37}$$

where p_{ns} and p_{d} are the pressure on the free-flow side and porous side of the interface, respectively, and $\mathbf{K}$ is the viscous stress tensor (defined only on the free-flow side).

For the coupling condition for the tangential velocity component, there are several options. One of the most widely used conditions is the **Beavers-Joseph** interface condition (Ref. 1):

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{u}_{ns} - \mathbf{u}_{d}) = \frac{\sqrt{\mathrm{tr}(\kappa)/n}}{\mu_{ns}\alpha_{BJ}}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n} \tag{7-38}$$

where α_{BJ} is the Beavers and Joseph parameter, κ is the permeability tensor of the porous medium (defined on the porous side of the interface), μ_{ns} is the fluid's dynamic viscosity on the free-flow side of the interface, and n is the number of space dimensions.

When the velocity in the porous domain is much smaller than the velocity in the free flow, one can use a modification of the Beavers–Joseph condition which is given by the **Beavers–Joseph–Saffman** interface condition (Ref. 2):

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{u}_{\mathrm{ns}} = \frac{\sqrt{\mathrm{tr}(\kappa)/n}}{\mu_{\mathrm{ns}}\alpha_{BJ}}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n} \tag{7-39}$$

For cases when the permeability tensor is not isotropic, the **Use projected permeability** option allows to take into account only the permeability in the direction of the tangential velocity component. This is accomplished by replacing the $\sqrt{\mathrm{tr}(\kappa)/n}$ term on the rights hand side of Equation 7-38 and Equation 7-39 by:

$$\sqrt{\mathbf{t} \cdot \kappa\mathbf{t}} \tag{7-40}$$

with $\mathbf{t}$ a unit vector tangent to the interface for 2D and 2D-axisymmetric cases, and for 3D cases by:

$$\sqrt{\mathbf{v} \cdot \kappa\mathbf{v}} \tag{7-41}$$

with $\mathbf{v}$ given by:

$$\mathbf{v} = \frac{(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n}}{\|(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n}\|} \tag{7-42}$$

If one considers the limit of the Beavers–Joseph condition for large values of the Beavers and Joseph parameter a_{BJ}, one obtains the **Continuous tangential velocity** condition:

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{u}_{\mathrm{ns}} - \mathbf{u}_{\mathrm{d}}) = 0 \tag{7-43}$$

The same limit for the Beavers–Joseph–Saffman condition results in the **No slip** condition:

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{u}_{\mathrm{ns}} = 0 \tag{7-44}$$

The **Viscous slip** condition allows for a more general coupling condition. This interface condition is given by:

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{u}_{\mathrm{ns}} - \mathbf{u}_{\mathrm{b}}) = \frac{L_s}{\mu_{\mathrm{ns}}}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n} \tag{7-45}$$

Here L_s is a slip length, and $\mathbf{u}_b$ a user-defined interfacial velocity.

Please find related information in the *CFD Module User's Guide*:

- The Darcy's Law Interface
- The Thin-Film and Porous Media Flow Interface
- The Laminar Flow Interface
- Theory for the Single-Phase Flow Interfaces

References

1. G.S. Beavers and D.D. Joseph, "Boundary Conditions at a Naturally Permeable Wall," *J. Fluid Mech.*, vol. 30, 1967.

2. P.G. Saffman, "On the Boundary Condition at the Surface of a Porous Medium," *Stud. Appl. Math.*, vol. 50, no. 2, pp. 93–101, 1971.

Theory for the Two-Phase Darcy's Law Interface

About the Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law interface combines Darcy's law (Equation 7-26) with the continuity equation (Equation 7-27) for the average density ρ. In the presence of two miscible fluid phases, the average density ρ and average viscosity μ depend on the composition of the mixture (Ref. 1). In the Two-Phase Darcy's Law interface these dependencies are given by

$$1 = s_1 + s_2 \tag{7-46}$$

$$\rho = s_1\rho_1 + s_2\rho_2 \tag{7-47}$$

$$\frac{1}{\mu} = s_1\frac{\kappa_{r1}}{\mu_1} + s_2\frac{\kappa_{r2}}{\mu_2} \tag{7-48}$$

Here, s_1 and s_2 represent the saturation of each phase, ρ_1 and ρ_2 the densities, and κ_{r1} and κ_{r2} the relative permeabilities. When either of the fluids is compressible, its density can be related to the pressure (for instance using the ideal gas law).

Beside the continuity equation for the mixture, the Two-Phase Darcy's Law interface also solves the transport equation for the fluid content of one of the phases, $c_1 = s_1\rho_1$:

$$\frac{\partial}{\partial t}(\varepsilon_p c_1) + \nabla \cdot (c_1\mathbf{u}) = \nabla \cdot D_c \nabla c_1 \tag{7-49}$$

Here, D_c (SI unit: m^2/s) is the capillary diffusion coefficient, which can be directly specified or derived from a capillary pressure expression. Normally, the fluid content c_1 will be the concentration of the wetting phase.

When *capillary pressure* is selected as capillary model, the capillary diffusion coefficient is computed from the saturation of one of the phases and the capillary pressure:

$$D_c = \frac{\kappa_{r1}}{\mu_1}\kappa(s_1 - 1)\frac{\partial p_c}{\partial s_1} \tag{7-50}$$

The capillary pressure is defined as the pressure difference between the phases, and it can be defined as a function of saturation, $p_c(s_1)$.

Capillary Pressure Models

The capillary pressure can be a user defined expression, or it can be derived from van Genuchten (Ref. 2) or Brooks and Corey (Ref. 3) models.

For van Genuchten model, the expression for the capillary pressure as a function of saturation follows the curve

$$p_c = p_{ec}\left(\frac{1}{s_1^{1/m}} - 1\right)^{1-m} \tag{7-51}$$

where p_{ec} is the entry capillary pressure and m is a constitutive exponent.

For the Brooks and Corey model, the capillary pressure curve depends on saturation as

$$p_c = p_{ec}\frac{1}{s_1^{1/\lambda}} \tag{7-52}$$

where λ is the pore distribution index.

When capillary pressure is selected as capillary model, the relative permeabilities are also determined by the van Genuchten or Brooks and Corey models. For the van Genuchten model, the relative permeabilities are given by

$$\kappa_{r1} = s_1^{l_{vG}}\left(1-\left(1-s_1^{1/m_{vG}}\right)^{m_{vG}}\right)^2$$

$$\kappa_{r2} = (1-s_1)^{l_{vG}}\left(1-s_1^{1/m_{vG}}\right)^{2m_{vG}}$$

where m_{vG} and l_{vG} are constitutive constants.

For the Brooks and Corey model, the relative permeabilities are given by

$$\kappa_{r1} = s_1^{(3+2/\lambda)}$$

$$\kappa_{r2} = (1-s_1)^2\left(1-s_1^{(1+2/\lambda)}\right)$$

where λ is again the pore distribution index.

References for the Two-Phase Darcy's Law Interface

1. Z. Chen, G. Huan, and Y. Ma, *Computational Methods for Multiphase Flows in Porous Media*. Philadelphia: Society for Industrial and Applied Mathematics, 2006.

2. M.Th. van Genuchten, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," *Soil Sci. Soc. Am. J.*, vol. 44, 1980.

3. R.H. Brooks and A.T. Corey, "Properties of Porous Media Affecting Fluid Flow," *J. Irrig. Drainage Div., ASCE Proc.*, vol. 72 (IR2), 1966.

Theory for the Multiphase Flow in Porous Media Interface

The model equations that are solved in the **Multiphase Flow in Porous Media** interface are based on the mass conservation of each phase and on an extended Darcy's law. The mass conservation equation for each phase is given by

$$\frac{\partial}{\partial t}(\varepsilon_p \rho_i s_i) + \nabla \cdot (\rho_i \mathbf{u}_i) = Q_i \tag{7-53}$$

where ε_p (dimensionless) is the porosity, and the vector $\mathbf{u}_i$ should be interpreted as the volumetric flux of phase i (SI unit $m^3/(m^2 \cdot s)$ or m/s). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_i = -\frac{\kappa_{ri}}{\mu_i}\kappa(\nabla p_i - \rho_i \mathbf{g}) \tag{7-54}$$

where κ denotes the permeability (SI unit: m^2) of the porous medium, $\mathbf{g}$ the gravitational acceleration vector (SI unit: m/s^2), and μ_i the dynamic viscosity (SI unit: $kg/(m \cdot s)$), p_i the pressure field (SI unit: Pa), and κ_{ri} the relative permeability (dimensionless) of phase i, respectively. The phase pressures p_i are related through the capillary pressure functions $p_{c_{ij}}$:

$$p_i - p_j = p_{c_{ij}}(s_1, \ldots, s_N) \qquad i \neq j \tag{7-55}$$

One phase pressure can be chosen independently so that $N - 1$ capillary pressure relations are needed to define the other phase pressures. In addition it is assumed that all phases together fill the pore space completely, so that we have

$$\sum_{i=1}^{N} s_i = 1 \tag{7-56}$$

Pressure-Saturation Formulation

The algebraic relations in Equation 7-55 and Equation 7-56 allow for a reduction of the number of dependent variables. An often used way is to eliminate $N - 1$ phase pressures and one of the saturations. This results in a so-called pressure-saturation

formulation (Ref. 3). The procedure in the **Multiphase Flow in Porous Media** interface is to pick one of the phases, let us say phase i_c, then express the volume fraction, or saturation, s_{i_c}, of this phase in terms of the saturations of the other phases and in addition to use the pressure, p_{i_c}, of this phase to define the other phase pressures:

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i \right) \tag{7-57}$$

$$p_i = p_{i_c} + p_{c_i}(s_1, \ldots, s_N) \qquad \text{for} \quad i \neq i_c \tag{7-58}$$

The equations for the saturations s_i, $(i \neq i_c)$ are given by Equation 7-53 and Equation 7-54. To arrive at an equation for p_{i_c}, the conservation equations of all phases are summed. This results in

$$\frac{\partial}{\partial t}\left(\varepsilon_p \sum_{i=1}^{N} \rho_i s_i \right) + \nabla \cdot \left(\sum_{i=1}^{N} \rho_i \mathbf{u}_i \right) = Q_{tot} \tag{7-59}$$

where the total mass source Q_{tot} is given by

$$Q_{tot} = \sum_{i=1}^{N} Q_i \tag{7-60}$$

The equations for the saturations s_i are solved in the **Phase Transport in Porous Media** interface (Equation 7-53 and Equation 7-54). The Equation 7-59 for the pressure field p_{i_c}, needed as an input to the **Phase Transport in Porous Media** interface, is solved for in the **Darcy's Law** interface: the **Multiphase Flow in Porous Media** multiphysics coupling interface replaces the equation

$$\frac{\partial}{\partial t}(\varepsilon_p \rho_{tot}) + \nabla \cdot (\rho_{tot} \mathbf{u}_d) = Q_m \quad \text{where} \quad \mathbf{u}_d = -\frac{1}{\mu}\kappa(\nabla p - \rho_{tot}\mathbf{g}) \tag{7-61}$$

which is originally implemented in the **Darcy's Law** interface, with Equation 7-59 by adding the following terms to the left-hand side of Equation 7-61:

$$\nabla \cdot \left(\sum_{i=1}^{N} \rho_i \mathbf{u}_i - \rho_{tot} \mathbf{u}_d \right) \tag{7-62}$$

and by setting the right-hand side Q_m to be equal to Q_{tot}. The volume averaged density ρ_{tot} is given by

$$\rho_{tot} = \sum_{i=1}^{N} \rho_i s_i \tag{7-63}$$

Furthermore, the **Multiphase Flow in Porous Media** multiphysics coupling interface couples the user inputs for the porosity and permeability of the porous matrix in the **Darcy's Law** interface to the corresponding user input fields in the **Phase and Porous Media Transport Properties** feature, and couples the pressure field computed for in the **Darcy's Law** interface to the user input field for the pressure of the phase computed from the volume constraint.

Note that when the hydraulic conductivity of a domain is specified in the **Darcy's Law** interface (instead of the permeability), the coupled **Phase and Porous Media Transport Properties** feature is supplied with a permeability that is computed using a reference kinematic viscosity of $1.004*10^{-6}$ $m^2 \cdot s^{-1}$ (kinematic viscosity of water at 293.15 K).

In the other direction, the multiphysics coupling node provides the averaged density (denoted by ρ_{tot} in Equation 7-62 above) and effective viscosity to the **Darcy's Law** interface.

Mass Source and Boundary Mass Source

When adding a Mass Source node in the coupled Phase Transport interface, it is by default assumed that the net mass source of all phases, Q_{tot}, equals zero. This implies

$$Q_{i_c} = -\sum_{i=1, i \neq i_c}^{N} Q_i \tag{7-64}$$

However, when mass is transferred from or to phases not accounted for in the phase transport interface — for instance, when mass is released or absorbed by the solid part of the porous matrix — select the **Mass transfer to other phases** checkbox. In this case the mass source for the phase calculated from the volume constraint should also be specified, and the net total mass source Q_{tot} is supplied as a right-hand side to the Darcy Equation 7-59 for p_{i_c} .

Similarly, when a Boundary Mass Source node is added in the coupled Phase Transport interface, the sum of the specified mass fluxes for all phases is supplied as a mass flux boundary condition for the Darcy Equation 7-59.

Boundary Conditions

When supplying boundary conditions for the coupled **Phase Transport in Porous Media** and **Darcy's Law** interfaces, bear in mind that the **Pressure** boundary condition in the **Darcy's Law** interface affects the pressure of the phase from the volume constraint, p_{i_c}. If the pressure of another phase needs to supplied, then take into account the capillary pressure.

Since the coupled **Darcy's Law** interface uses the conservation equation for the total mass (Equation 7-59) to solve for p_{i_c}, the **Mass Flux** boundary condition in the **Darcy's Law** interface should be used to prescribe the mass flux of all phases together.

If the mass flux of the phase computed from the volume constraint needs to be prescribed at a boundary, and the total mass flux is not known a priori, it might be necessary to compute for the total mass flux in the form of a Lagrange multiplier by using the weak constraint formulation for the pressure boundary condition in the **Darcy's Law** interface.

Thin Barrier (Multiphysics Coupling)

The **Thin Barrier** multiphysics coupling uses the Extra Dimension tool to solve the equations for the pressure and saturations through the thin barrier structure's thickness. The thin structure has its domain represented by the product space between the lumped boundary and the additional dimension for the thickness. Inside this product space, it is convenient to split the gradient operator into a tangential part and a normal part: $\nabla=\nabla_{\mathbf{t}}+\nabla_{\mathbf{n}}$.

The following assumptions, used in deriving the **Thin Barrier** equations from the equations solved in the **Multiphase Flow in Porous Media** interface, justify the simplification $\nabla=\nabla_{\mathbf{n}}$:

- A thin barrier can be considered as a boundary of thickness significantly smaller than the typical lengths of the overall model.
- The permeability of the porous material inside the thin barrier is significantly smaller than the permeability of the porous material in the adjacent domains.
- There is no mass source or sink inside the thin barrier.

In addition, these assumptions imply that the effect of gravity on the phase transport can be neglected. This results in the following set of equations for the saturations s_i, $(i \neq i_c)$ and the pressure p_{i_c} :

$$\frac{\partial}{\partial t}(\varepsilon_p \rho_i s_i) + \nabla_{\mathbf{n}} \cdot (\rho_i \mathbf{u}_i) = 0 \quad \text{for} \quad i \neq i_c \tag{7-65}$$

$$\mathbf{u}_i = -\frac{\kappa_{ri}}{\mu_i} \kappa \nabla_{\mathbf{n}} p_i \tag{7-66}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_p \sum_{i=1}^{N} \rho_i s_i \right) + \nabla_{\mathbf{n}} \cdot \left(\sum_{i=1}^{N} \rho_i \mathbf{u}_i \right) = 0 \tag{7-67}$$

Together with the algebraic relations

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i \right) \tag{7-68}$$

$$p_i = p_{i_c} + p_{c_i}(s_1, \ldots, s_N) \qquad \text{for} \quad i \neq i_c \tag{7-69}$$

Here ε_p (dimensionless) denotes the porosity and κ the permeability (SI unit: m^2) of the porous material in the thin barrier. Further more ρ_i denotes the density (SI unit: kg/m^3), μ_i the dynamic viscosity (SI unit: kg/(m·s)), p_i the pressure field (SI unit: Pa), $\mathbf{u}_i$ the (normal) volumetric flux (SI unit: m/s) and κ_{ri} the relative permeability (dimensionless) of phase i, respectively.

Since the interfaces between the thin barrier and the adjacent domains are boundaries between a more permeable and a less permeable porous domain, conditions analogous to the Porous Medium Discontinuity Boundary Condition are needed to couple the equation Equation 7-65 for the saturations inside the thin barrier to the equations in the adjacent domains. These condition at the extremities of the extra dimension can be written as:

$$p^t_{c_i}(s^t_i)_{L=0} = \begin{cases} p^t_{ec,\,i} & \text{if} \quad p^d_{c_i}(s^d_i) \leq p^t_{ec,\,i} \\ p^d_{c_i}(s^d_i) & \text{if} \quad p^d_{c_i}(s^d_i) > p^t_{ec,\,i} \end{cases} \qquad \text{for} \quad i \neq i_c \tag{7-70}$$

where the superscript t is used to indicate the saturation and capillary pressure inside the thin barrier (the low permeable side of the interface), and the superscript d

indicates the domain adjacent to the downside of the thin barrier (the high permeable side), and

$$p_{c_i}^t(s_i^t)_{L=d_s} = \begin{cases} p_{ec,i}^t & \text{if} \quad p_{c_i}^u(s_i^u) \le p_{ec,i}^t \\ p_{c_i}^u(s_i^u) & \text{if} \quad p_{c_i}^u(s_i^u) > p_{ec,i}^t \end{cases} \quad \text{for} \quad i \ne i_c \qquad (7\text{-}71)$$

where the superscript u indicates the domain adjacent to the upside of the thin barrier (again the high permeable side) and where d_s is the length of the extra dimension, or equivalently, the thickness of the thin structure.

The additional conditions are continuity of the fluxes for all phases and continuity of the pressure of the phase i_c computed from the volume constraint. Note that this last condition assumes that this phase is present both inside the thin barrier and in the adjacent domains. Furthermore, this boundary condition assumes that the phase i_c computed from the volume constraint is the wetting phase and it is necessary that the settings for the van Genuchten or Brooks and Corey capillary pressure model in the adjacent domains match this assumption.

Please find related information under

- Theory for the Phase Transport Interfaces in the *CFD Module User's Guide* and
- Using Extra Dimensions in the *COMSOL Multiphysics Reference Manual*.

References

1. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing, 1972.

2. Z. Chen, G. Huan, and Y. Ma, *Computational Methods for Multiphase Flows in Porous Media*, Philadelphia: Society for Industrial and Applied Mathematics, 2006.

3. R. Helmig, *Multiphase Flow and Transport Processes in the Subsurface – A Contribution to the Modeling of Hydrosystems*, Springer–Verlag, 1997.

Theory for the Thin-Film and Porous Media Flow Interface

No-Slip Condition

The no-slip condition ensures that the total pressure in the porous media, $p + p_{\text{ref}}$, matches the total pressure in the thin-film region, $p_{\text{film}} + p_{\text{ref}}$, at the intersection of the physics interfaces, that is,

$$p_{\text{film}} + p_{\text{ref}} = p + p_{\text{ref}}. \tag{7-72}$$

Also, a mass source/sink term is added to the Reynolds equation or the modified Reynolds equation that accounts for mass flux at the interface. For Reynolds equation, it takes the form

$$Q = \rho(\mathbf{u} \cdot \mathbf{n}), \tag{7-73}$$

and, for the modified Reynolds equation, it takes the form

$$Q = p_A(\mathbf{u} \cdot \mathbf{n}), \tag{7-74}$$

where, $\mathbf{n}$ is the normal to the interface, ρ is the fluid density, p_A is the total pressure and $\mathbf{u}$ is the fluid velocity in the porous media at the interface.

Beavers–Joseph Slip Condition

In addition to the pressure balance given in Equation 7-72 and consideration for mass flux across the interface in Equation 7-73 and Equation 7-74, the Beavers–Joseph slip condition models the development of the boundary layer at the intersection of the physics interfaces using a small interface slip velocity.

The condition ensures that the tangential velocity at the interface is continuous when the slip velocity is included at the wall and base boundaries of the thin-film region. The slip length parameter accounts for the slip velocity, as given in Equation 9-9 in the *CFD Module Reference Manual*. Depending on the orientation of the interface normal with respect to the reference surface normal, the expressions are given as

$$\mathbf{v}_{w,t} = \text{down}(\mathbf{u}_t), \text{ if } \mathbf{n} = \mathbf{n}_{\text{ref}}. \ \mathbf{v}_{w,t} = \text{up}(\mathbf{u}_t), \text{ if } \mathbf{n} = -\mathbf{n}_{\text{ref}}. \tag{7-75}$$

$$\mathbf{v}_{b,t} = \text{up}(\mathbf{u}_t), \text{ if } \mathbf{n} = \mathbf{n}_{\text{ref}}. \ \mathbf{v}_{b,t} = \text{down}(\mathbf{u}_t), \text{ if } \mathbf{n} = -\mathbf{n}_{\text{ref}}., \tag{7-76}$$

$$L_{sw} = \frac{\sqrt{\text{tr}(\text{down}(\kappa))}}{\alpha_{\text{BJ,w}}}, \text{ if } \mathbf{n} = \mathbf{n}_{\text{ref}}. \ L_{sw} = \frac{\sqrt{\text{tr}(\text{up}(\kappa))}}{\alpha_{\text{BJ,w}}}, \text{ if } \mathbf{n} = -\mathbf{n}_{\text{ref}}. \tag{7-77}$$

$$L_{sb} = \frac{\sqrt{\text{tr}(\text{up}(\kappa))}}{\alpha_{\text{BJ,b}}}, \text{ if } \mathbf{n} = \mathbf{n}_{\text{ref}}. \ L_{sb} = \frac{\sqrt{\text{tr}(\text{down}(\kappa))}}{\alpha_{\text{BJ,b}}}, \text{ if } \mathbf{n} = -\mathbf{n}_{\text{ref}}. \tag{7-78}$$

Here, tr() is the trace operator, κ is the permeability tensor of the porous media, $\mathbf{v}$ is the thin-film velocity, subscripts b and w represent the base and wall boundaries of the thin-film region, respectively, and the subscript t represents the component tangential to the interface.

References for the Thin-Film and Porous Media Flow Interface

1. H. Wu, "An Analysis of the Squeeze Film Between Porous Rectangular Plates," *J. Lubr. Technol.*, vol. 94, no. 1, pp. 64–68, 1972.

2. J. Prakash and S. K. Vij, "Analysis of Narrow Porous Journal Bearing Using Beavers-Joseph Criterion of Velocity Slip," *J. Appl. Mech.*, vol. 41, no. 2, pp. 348–354, 1974.

8

Chemical Species Transport Interfaces

The physics interfaces under the **Chemical Species Transport** branch ( ) accommodate all types of material transport that can occur through diffusion and convection. The section Modeling Chemical Species Transport helps you choose the best physics interface to start with.

In this chapter:

- The Transport of Diluted Species Interface
- The Transport of Diluted Species in Porous Media Interface
- The Transport of Concentrated Species Interface
- The Transport of Concentrated Species in Porous Media Interface
- The Vapor Flow Multiphysics Interfaces
- The Reacting Flow, Concentrated Species Multiphysics Interfaces
- The Reacting Flow, Diluted Species Multiphysics Interfaces
- The Reacting Flow in Porous Media Interfaces
- The Nonisothermal Reacting Flow Multiphysics Interfaces
- The High Mach Number Reacting Flow Multiphysics Interfaces
- The High Mach Number Reacting Flow, Diluted Species Multiphysics Interfaces

- The Dispersed Two-Phase Flow with Species Transport Multiphysics Interfaces
- Theory for the Transport of Diluted Species Interface
- Theory for the Transport of Concentrated Species Interface
- Theory for the Reacting Flow Interfaces

Modeling Chemical Species Transport

In this section:

- Selecting the Right Physics Interface
- Coupling to Other Physics Interfaces
- Adding a Chemical Species Transport Interface

Selecting the Right Physics Interface

The behavior of chemical reactions in real environments is often not adequately described by the assumptions of perfectly mixed or controlled environments. This means that the transport of material through both time and space need to be considered. Physics interfaces in the **Chemical Species Transport** branch accommodate all types of material transport that can occur through diffusion and convection — either alone or in combination with one another. The branch includes physics interfaces solving equations for diluted as well as concentrated mixtures, where the species propagation can occur in solids, free flowing fluids, or through porous media.

The Transport of Diluted Species Interface ( ) is applicable for solutions (either fluid or solid) where the transported species have concentrations at least one order of magnitude less than the solvent. The settings for this physics interface can be chosen to simulate chemical species transport through diffusion (Fick's law) and convection (when coupled to fluid flow).

The Transport of Concentrated Species Interface ( ) is used for modeling transport within mixtures where no single component is clearly dominant. Often the concentrations of the participating species are of the same order of magnitude, and the molecular effects of the respective species on each other need to be considered. This physics interface supports transport through Fickian diffusion, a mixture average diffusion model, and as described by the Maxwell-Stefan equations.

REACTING FLOW

The Reacting Laminar Flow, Concentrated Species Interface ( ) combines the functionality of the Laminar Flow and Transport of Concentrated Species interfaces. Using this physics interface the mass and momentum transport in a reacting fluid can be modeled, with the couplings between the velocity field and the mixture density set

up automatically. This physics interface is applicable for fluid flow in the laminar regime.

The Reacting Turbulent Flow, k-ε, Concentrated Species Interface ( ) combines the functionality of the Turbulent Flow, k-ε and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the standard k-ε model, solving for the turbulent kinetic energy k and the rate of dissipation of turbulent kinetic energy ε.

The Reacting Turbulent Flow, k-ω, Concentrated Species Interface ( ) combines the functionality of the Turbulent Flow, k-ω and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the Wilcox revised k-ω model, solving for the turbulent kinetic energy k and the rate of specific dissipation of turbulent kinetic energy ω.

The Reacting Turbulent Flow, SST, Concentrated Species Interface ( ) combines the functionality of the Turbulent Flow, SST and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the Menter SST model, solving for the turbulent kinetic energy k and the rate of specific dissipation of turbulent kinetic energy ω. The physics interface also includes a wall distance equation that solves for the reciprocal wall distance.

The Reacting Turbulent Flow, Low Re k-ε, Concentrated Species Interface ( ) combines the functionality of the Turbulent Flow, Low Re k-ε and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the AKN low-Reynolds

number k-ε model, solving for the turbulent kinetic energy k and the rate of dissipation of turbulent kinetic energy ε. The physics interface also includes a wall distance equation that solves for the reciprocal wall distance.

REACTING FLOW IN POROUS MEDIA

The Reacting Flow in Porous Media, Transport of Diluted Species Interface ( ) merges the functionality of the Transport of Diluted Species and the Free and Porous Media Flow interfaces into a multiphysics interface. This way, coupled mass and momentum transport in free and porous media can be modeled from a single physics interface, with the nonlocal coupling for the velocity field set up automatically. In addition, the effective transport coefficients in a porous matrix domain can be derived based on the corresponding values in for a nonporous domain.

The Reacting Flow in Porous Media, Transport of Concentrated Species Interface ( ) combines the Transport of Concentrated Species and the Free and Porous Media Flow interfaces. This means that mass and momentum transport can be modeled from a single physics interface, with the couplings between the velocity field and the mixture density set up automatically. Also, the effective transport coefficients in a porous matrix domain are derived based on the corresponding values for a nonporous domain. This physics interface is applicable for fluid flow in the laminar regime.

HIGH MACH NUMBER REACTING FLOW

The High Mach Number Reacting Laminar Flow Interface ( ) combines the functionality of the High Mach Number Laminar Flow interface, the Transport of Concentrated Species interface and optionally, the Chemistry interface for modeling transport and reaction of species in gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range. The High Mach Number Reacting Flow multiphysics coupling, added automatically, couples the velocity field and takes into account the heat of reaction, enthalpy diffusion and contributing mass fluxes.

The High Mach Number Reacting Turbulent Flow, k-ε Interface ( ) combines the functionality of the High Mach Number Flow, k-ε interface, the Transport of Concentrated Species interface and optionally, the Chemistry interface for modeling transport and reaction of species in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range. The High Mach Number Reacting Flow multiphysics coupling, added automatically, couples the velocity field, takes into account the heat of reaction, enthalpy diffusion and contributing mass fluxes, and introduces mass transport turbulence modeling.

The High Mach Number Reacting Turbulent Flow, Spalart–Allmaras Interface ( ) combines the functionality of the High Mach Number Flow, Spalart–Allmaras interface, the Transport of Concentrated Species interface and optionally, the Chemistry interface for modeling transport and reaction of species in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range. The High Mach Number Reacting Flow multiphysics coupling, added automatically, couples the velocity field, takes into account the heat of reaction, enthalpy diffusion and contributing mass fluxes, and introduces mass transport turbulence modeling.

HIGH MACH NUMBER REACTING FLOW, DILUTED SPECIES

The High Mach Number Reacting Laminar Flow, Diluted Species Interface ( ) combines the functionality of the High Mach Number Laminar Flow and the Transport of Diluted Species interfaces for modeling mass transport of species dissolved in gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range. The High Mach Number Reacting Flow, Diluted Species multiphysics coupling, added automatically, couples the velocity field.

The High Mach Number Reacting Turbulent Flow, k-ε, Diluted Species Interface ( ) combines the functionality of the High Mach Number Flow, k-ε and the Transport of Diluted Species interfaces for modeling mass transport of species dissolved in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range. The High Mach Number Reacting Flow, Diluted Species multiphysics coupling, added automatically, couples the velocity field, adds turbulent mixing contributions to the mass transport equations and introduces mass transport turbulence modeling.

The High Mach Number Reacting Turbulent Flow, Spalart–Allmaras, Diluted Species Interface ( ) combines the functionality of the High Mach Number Flow, Spalart–Allmaras and the Transport of Diluted Species interfaces for modeling mass transport of species dissolved in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range. The High Mach Number Reacting Flow, Diluted Species multiphysics coupling, added automatically, couples the velocity field, adds turbulent mixing contributions to the mass transport equations and introduces mass transport turbulence modeling.

Coupling to Other Physics Interfaces

When you are simulating applications that can be described by the material transport interfaces in the **Chemical Species Transport** branch, there is often a need to couple the material transport to other physics interfaces. Convection is often the cause of the material transport, so couplings to Fluid Flow interfaces is required. The CFD Module includes physics interfaces for Laminar Flow and Porous Media Flow as well as more advanced descriptions of fluid flow, such as turbulent and Multiphase Flow.

Moreover, most chemical reactions or other types of material processing, such as casting, either require or produce heat, which in turn affects both the reaction and other physical processes connected to the system. This module includes physics interfaces for heat transfer through conduction and convection as well as through porous media. More extensive description of heat transfer, such as surface-to-surface radiation, can be found in the Heat Transfer Module.

Finally, COMSOL Multiphysics supports simulations of electrostatics or DC-based physical phenomena, even when the conductivity is nonlinear. If the electric field is AC/DC in nature, or if your system is affected by electromagnetic waves, then the AC/DC Module and RF Module include appropriate physics interfaces for such phenomena. Furthermore, some applications of electrochemical reactions, particularly in electrochemical power source applications, are better handled by the Battery Design Module.

Adding a Chemical Species Transport Interface

A chemical species transport interface can be added when first creating a new model, or at any time during the modeling process.

Creating a New Model in the *COMSOL Multiphysics Reference Manual*

1 To add a physics interface:

- Select **New** to open the **Model Wizard**, after selecting a space dimension, go to the **Select Physics** page.
- From the **Home** toolbar, click **Add Physics** ( ). Or right-click the **Component** node in the **Model Builder** and select **Add Physics**. Go to the **Add Physics** window.

2 Under **Chemical Species Transport**, navigate to the physics interface to add and double-click it.

There are other ways to add a physics interface depending on whether you are in the Model Builder or Add Physics window:

- In the **Model Wizard**, click **Add** or right-click and select **Add Physics** (+). The physics interface displays under **Added physics interfaces**.
- In the **Add Physics** window, click **Add to Component** (+) or right-click and select **Add to Component**.

3 Specify the number of species (concentrations or mass fractions) and the names:

- In the **Model Wizard**, on the **Review Physics Interface** page under **Dependent Variables**.
- In the **Add Physics** window, click to expand the **Dependent Variables** section.
- After adding the physics interface, you can also edit this information — click the node in the **Model Builder**, then, in the **Settings** window under **Dependent Variables**, specify the information.

4 Continue by adding more interfaces and specifying the number of species (concentrations or mass fractions) that are to be simulated in a mass transport physics interface when adding that interface.

5 In the **Dependent Variables** section, enter the **Number of species**. To add a single species, click the **Add Concentration** button (+) underneath the table or enter a value into the **Number of species** field. Click the **Remove Concentration** button ( ) underneath the table if required.

The **Transport of Concentrated Species** interface needs to contain at least two species (the default). Also edit the strings or names directly in the table. The names must be unique for all species (and all other dependent variables) in the model.

The Transport of Diluted Species Interface

The **Transport of Diluted Species (tds)** interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid, or solid can be handled with this interface. The driving forces for transport can be diffusion by Fick's law, convection when coupled to a flow field, and migration, when coupled to an electric field.

The interface supports simulation of transport by convection and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, c_i, of each species i.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tds`.

DOMAIN SELECTION

If any part of the model geometry should not partake in the mass transfer model, remove that part from the selection list.

OUT-OF-PLANE THICKNESS

For 2D components, the **Thickness** field (default value: 1 m) defines a parameter for the thickness of the geometry perpendicular to the two-dimensional cross-section. Both constant and varying thicknesses are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux.

CROSS-SECTIONAL AREA

For 1D components, enter a **Cross-sectional area** A_c (SI unit: m^2) to define a parameter for the area of the geometry perpendicular to the 1D component. Both constant and varying areas are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux. The default is 1 m^2.

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the checkboxes available under **Additional transport mechanisms** to control other transport mechanisms.

Note: Some of the additional transport mechanisms listed below are only available in certain products. For details see https://www.comsol.com/products/specifications/.

- By default, the **Convection** checkbox is selected. Clear the checkbox to disable convective transport.
- Select the **Migration in electric field** checkbox to activate transport of ionic species in an electric field. See further the theory section Adding Transport Through Migration.

Transport of ionic species in an electric field is available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Mass Transport in Porous Media

The **Mass transport in porous media** checkbox activates functionality specific to species transport in porous media:

- Porous Medium
- Unsaturated Porous Medium
- Porous Electrode Coupling
- Volatilization
- Species Source

Note: Mass transport in porous media is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

CONSISTENT STABILIZATION

To display this sections, click the **Show** button ( ) and select **Stabilization**.

- When the **Crosswind diffusion** checkbox is selected, a weak term that reduces spurious oscillations is added to the transport equation. The resulting equation system is always nonlinear. There are two options for the **Crosswind diffusion type**:
  - **Do Carmo and Galeão** — the default option. This type of crosswind diffusion reduces undershoots and overshoots to a minimum but can in rare cases give equation systems that are difficult to fully converge.
  - **Codina** — this option is less diffusive compared to the Do Carmo and Galeão option but can result in more undershoots and overshoots. It is also less effective for anisotropic meshes. The Codina option activates a text field for the **Lower gradient limit** g_{lim}. Its defaults to `0.1[mol/m^3]/tds.helem`, where `tds.helem` is the local element size.
- For both consistent stabilization methods, select an **Equation residual**. **Approximate residual** is the default and means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is computationally faster. If required, select **Full residual** instead.

INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**. By default, the **Isotropic diffusion** checkbox is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for under resolved problems.

ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed. Select a **Material Balance Form** — **Nonconservative** (the default) or **Conservative**. The conservative formulation should be used for compressible flow. See Material Balance Formulation for more information.

DISCRETIZATION

To display all settings available in this section, click the **Show** button ( ) and select **Advanced Physics Options**.

The **Compute boundary fluxes** checkbox is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the checkbox is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

The flux variables affected in the interface are:

- `ndflux_`*c* (where *c* is the dependent variable for the concentration). This is the normal diffusive flux and corresponds to the boundary flux when diffusion is the only contribution to the flux term.
- `ntflux_`*c* (where *c* is the dependent variable for the concentration). This is the normal total flux and corresponds to the boundary flux plus additional transport terms, for example, the convective flux when you use the nonconservative form.

Also the **Apply smoothing to boundary fluxes** checkbox is available if the previous checkbox is selected. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the *COMSOL Multiphysics Reference Manual*.

The **Value type when using splitting of complex variables** setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variable name is the **Concentration** *c* by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the **Number of species**. Use the **Add concentration** (+) and **Remove concentration** ( ) buttons as needed.

FURTHER READING

- Theory for the Transport of Diluted Species Interface
- Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*.
- In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

- *Effective Diffusivity in Porous Materials*: Application Library path **COMSOL_Multiphysics/Diffusion/effective_diffusivity**
- *Micromixer*: Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/micromixer**

The Transport of Diluted Species in Porous Media Interface

This interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the species concentration and transport in free and porous media. The interface is the same as the *Transport of Diluted Species* interface but it uses other defaults: The Mass Transport in Porous Media property is selected, and a Porous Medium node is added by default. The interface includes reaction rate expressions and solute sources for modeling of species transport and reaction in porous media.

This interface is dedicated to modeling transport in porous media, including immobile and mobile phases, where the chemical species may be subjected to diffusion, convection, migration, dispersion, adsorption, and volatilization in porous media. It supports cases where either the solid phase substrate is exclusively immobile, or when a gas-filling medium is also assumed to be immobile.

It applies to one or more diluted species or solutes that move primarily within a fluid that fills (saturated) or partially fills (unsaturated) the voids in a solid porous medium. The pore space not filled with fluid contains an immobile gas phase. Models including a combination of porous media types can be studied.

The main feature nodes are the **Porous Medium** and **Unsaturated Porous Medium** nodes, which add the equations for the species concentrations and provide an interface for defining the properties of the porous media, as well as additional properties governing

adsorption, volatilization, dispersion and diffusion, migration, and the velocity field to model convection.

The physics interface can be used for stationary and time-dependent analysis.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Porous Medium**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, reaction rate expressions, and species sources. You can also right-click **Transport of Diluted Species in Porous Media** to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as The Transport of Diluted Species Interface.

FURTHER READING

- Mass Balance Equation for Transport of Diluted Species in Porous Media
- Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

- *Variably Saturated Flow and Transport — Sorbing Solute*: Application Library path **Subsurface_Flow_Module/Solute_Transport/sorbing_solute**

  Web link: https://www.comsol.com/model/variably-saturated-flow-and-transport-sorbing-solute-490

Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar

(Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- To add a node, go to the **Physics** toolbar, no matter what operating system you are using.
- Contextual subnodes (attributes) are available by clicking the parent node in the Model Builder, and then selecting the subnode from the **Attributes** menu.

- Adsorption
- Concentration
- Continuity on Interior Boundaries
- Dispersion
- Electrode Surface Coupling
- Equilibrium Reaction
- Fast Irreversible Surface Reaction
- Fluid
- Fluid (Porous Medium)
- Flux
- Flux Discontinuity
- Fracture
- Gas
- Inflow
- Initial Values
- Line Mass Source
- Liquid
- Mass-Based Concentrations
- No Flux
- Open Boundary
- Out-of-Plane Flux
- Outflow
- Partition Condition
- Periodic Condition
- Point Mass Source
- Porous Matrix
- Porous Medium
- Porous Electrode Coupling
- Reaction Coefficients
- Reactions
- Solid
- Species Properties
- Species Source
- Surface Reactions
- Surface Equilibrium Reaction
- Symmetry
- Thin Diffusion Barrier
- Thin Impermeable Barrier
- Unsaturated Porous Medium
- Volatilization

Some features require certain add-on modules. For details see https://www.comsol.com/products/specifications/

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on boundaries representing the symmetry axis.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Prescribing Conditions on Fluid-Solid Interfaces

Defining conditions on interfaces between different phases, typically a wall in contact with a fluid, it is worthwhile to be careful with how variables in the conditions are evaluated. COMSOL Multiphysics supports that variables are defined differently on adjacent domains (or any other geometry dimension). Evaluating a variable with differing definitions, the mean value is returned on a boundary separating the different domains. The density, pressure, or temperature are examples of variables that may differ in a fluid and a solid. In order to specify on which side a variable is evaluated, the up and down operators (described in the *COMSOL Multiphysics Reference Manual*) can be used.

Species Properties

Use this node to define parameters specific to each of the species. It is available when the **Migration in electric field** checkbox is selected in the Transport Mechanisms section of the interface.

The node will change its label depending on what inputs are available in the node. If only **Charge** is available, it will be labeled “Species charges”.

CHARGE

Enter the charge number z_c (dimensionless, but requires a plus or minus sign) for each species.

ACTIVITY

This section is available when the **Species Activity** combo box is set to **Debye–Hückel** or **User defined**.

If **Debye–Hückel** is selected, enter the ion size number, a_0, for each species. If **User defined** is selected, enter the activity coefficient, f, for each species.

Fluid

The settings in this node are dependent on the checkboxes selected under Transport Mechanisms in the **Settings** window for the Transport of Diluted Species interface. It includes only the sections required by the activated transport mechanisms. It has all the equations defining transport of diluted species as well as inputs for the material properties.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select diffusion coefficients defined in a material or a Chemistry interface.

Select **Material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Fluid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All

defined diffusion coefficients are available for selection in the **Fluid diffusion coefficient** list.

For **User defined**, enter a value or expression for the **Fluid diffusion coefficient** D_c of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected. From the **Electric potential** list, select the source of the electric field.

- Enter a value or expression for the **Electric potential** V, which is **User defined**; this input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has also been added to the model.
- Select the electric potential defined or solved by Electrochemistry interface that has been added to the component.

By default the **Mobility** is set to be calculated based on the species diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, and under **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value of expression of the mobility $u_{m,c}$.

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based on the Nernst–Einstein relation) is taken from **Model Inputs** section.

Note that the migration in electric fields feature is only available in some COMSOL products. See details: https://www.comsol.com/products/specifications/.

EXAMPLE MODELS

	• *Separation Through Dialysis*: Application Library path **Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis** Web link: https://www.comsol.com/model/separation-through-dialysis-258

	• *Transport in an Electrokinetic Valve*: Application Library path **Microfluidics_Module/Fluid_Flow/electrokinetic_valve** Web link: https://www.comsol.com/model/transport-in-an-electrokinetic-valve-603

Solid

Use this node to describe diffusion in a solid phase domain. In this feature, the activities of the species are assumed to be ideal.

DIFFUSION

Specify the diffusion coefficients describing the diffusion of each species in the solid.

Enter a value or expression for the **Diffusion coefficient** D_c of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, or **Symmetric** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

ADVANCED

This section is only available with the **Advanced Physics Options** selected and when the model contains a split between the material frame and the spatial frame. A split of these frames occurs when using a **Moving Mesh** node or a Structural Mechanics interface like **Solid Mechanics**. In such a model, the reference geometry (the material frame) differs from the deformed geometry (the spatial frame). The diffusive transport of species is solved for on the material frame, but the equation is adjusted for geometry deformations so that species conservation is achieved on the spatial frame. Use the **Diffusion model** to define the frame of reference for the diffusion tensor.

Select **Reference geometry based (Lagrangian)** to specify the diffusion tensor in the undeformed geometry, implying that the diffusion is defined in the material frame

(indicated by coordinates X, Y, Z). This is the preferred setting for an anisotropic diffusion in combination with solid body translation or rotation. Also in general when the diffusion tensor components have been measured in an undeformed geometry.

Select **Deformed geometry based (Eulerian)** to specify the diffusion tensor in the deformed geometry. This means that the diffusion is defined in the spatial frame (indicated by coordinates x, y, z). Use this setting when the diffusion tensor components have been measured in a deformed geometry.

The **Advanced Physics Options** is found in the **Show More Options** dialog, accessed by clicking the **Show More Options** button ( ).

Note that multiple species are only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

Initial Values

The **Initial Values** node specifies the initial values for the concentration of each species. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

INITIAL VALUES

Enter a value or expression for the initial value of the **Concentration** or concentrations, c_i. This also serves as a starting guess for stationary problems.

Mass-Based Concentrations

Use the **Mass-Based Concentrations** node to add postprocessing variables for mass-based concentrations (SI unit: $\mathrm{kg/m^3}$) and mass fractions (dimensionless) for all species.

MIXTURE PROPERTIES

The default **Solvent density** ρ_{solvent} is taken **From material**. For **User defined**, enter a value or expression manually. Define the **Molar mass** of each species, which is needed to calculate the mass-based concentration.

Reactions

Use the **Reactions** node to account for the consumption or production of species through chemical reactions. Define the rate expressions as required.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

REACTION RATES

Add a rate expression R_i (SI unit: mol/(m^3·s)) for species i. Enter a value or expression in the field. Note that if you have the *Chemistry* interface available, provided with the *Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down lists. For an example, see the application *Fine Chemical Production in a Plate Reactor* as linked below.

REACTING VOLUME

This section is only available when the Mass Transport in Porous Media property is available and selected. See https://www.comsol.com/products/specifications/ for more details on availability.

When specifying reaction rates for a species in porous media, the specified reaction rate may have the basis of the total volume, the pore volume, or in the case of using the volume of a particular phase (applicable when modeling an unsaturated porous medium).

- For **Total volume**, the reaction expressions, in mol/(m^3·s), are specified per unit volume of the model domain (multiplied by unity).
- For **Pore volume**, the reaction expressions, in mol/(m^3·s), are specified per unit volume of total pore space. The reaction expressions will be multiplied by the domain porosity, ε_p. (ε_p equals unity for nonporous domains).
- For **Liquid phase**, the reaction expressions, in mol/(m^3·s), are specified per unit volume of liquid in the pore space. The expressions will be multiplied by the liquid volume fraction θ_l. (θ_l equals the porosity (ε_p) on Porous Medium domains).
- For **Gas phase**, the reaction expressions, in mol/(m^3·s), are multiplied by the gas volume fraction $\theta_g = \varepsilon_p - \theta_l$. θ_g equals 0 for Porous Medium domains.

FURTHER READING

See the theory chapter on chemical species transport, starting with the section *Mass Balance Equation*.

- *Fine Chemical Production in a Plate Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/ Reactors_with_Mass_and_Heat_Transfer/plate_reactor**

  Web link: https://www.comsol.com/model/fine-chemical-production-in-a-plate-reactor-8589

No Flux

This node is the default boundary condition on exterior boundaries. It should be used on boundaries across which there is no mass flux, typically solid walls where no surface reactions occur. The condition applied for each species corresponds to

$$-\mathbf{n} \cdot (-D\nabla c) = 0$$

where $\mathbf{n}$ denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the no flux condition is:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi) = 0$$

CONVECTION

By default, the feature prescribes a vanishing flux due to diffusion and migration in an electric field. This is the appropriate no flux condition when the relative convective velocity at the boundary is zero. When the fluid velocity at the boundary is not equal to that of the boundary, it is often convenient to prescribe the total flux including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the no flux condition prescribed is

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = 0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi + \mathbf{u}c) = 0$$

when migration of ionic species is included.

Inflow

Use this node to specify all species concentrations at an inlet boundary.

If you want to specify the concentration of a subset of the partaking species, this can be done by using the Concentration node instead.

For the **Electroanalysis** interface, this node is available when you select the **Convection** checkbox on the physics interface **Settings** window.

CONCENTRATION

For the concentration of each species $c_{0,c}$ (SI unit: mol/m^3), enter a value or expression.

BOUNDARY CONDITION TYPE

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints.

The other option, **Flux (Danckwerts)** can be used when the concentration at the boundary is not known, or when it varies in a nontrivial manner. This may, for example, be useful when reactions with high reaction rates occur in the vicinity of the inlet. In this case the concentration far upstream of the boundary is instead prescribed. The **Flux (Danckwerts)** condition prescribes the total flux defined by the upstream concentration and the fluid velocity at the boundary.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual.*

FURTHER READING

See the theory chapter in the section Danckwerts Inflow Boundary Condition.

Outflow

Apply this condition at outlets boundaries where species should be transported out of the model domain by fluid motion or by an electric field (in the case of ions). It is assumed that convection and migration (in an electric field) are the dominating transport mechanisms across the boundary, and therefore that the diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D\nabla c) = 0$$

Note that the **Convection** or the **Migration in electric field** transport mechanisms needs to be included for this node to be available.

Concentration

This condition node adds a boundary condition for the species concentration. For example, a $c = c_0$ condition specifies the concentration of species c.

CONCENTRATION

Individually specify the concentration for each species. Select the checkbox for the **Species** to specify the concentration, and then enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the checkbox for the concentration of that species.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

Flux

This node can be used to specify the species molar flux across a boundary. The flux can for example occur due to chemical reactions or a phase change at the boundary. The flux can also represent the transport to or from a surrounding environment currently not included model.

The prescribed flux of a species c is by default defined as

$$-\mathbf{n} \cdot (-D\nabla c) = J_0$$

where $\mathbf{n}$ denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi) = J_0$$

The flux prescribed, J_0, can include any arbitrary user-specified expression. It can be constant or a function of a dependent variable or independent variable. Common examples are a flux dependent of the concentration, temperature, pressure, or the electric potential ϕ.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

CONVECTION

By default, the flux due to diffusion and migration in an electric field is prescribed. This is the appropriate flux condition when the relative velocity at the boundary is zero. When the fluid velocity is not equal to that of the boundary, it is often convenient to prescribe the total flux, including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the prescribed flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = J_0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi + \mathbf{u}c) = J_0$$

when migration of ionic species is included.

INWARD FLUX

Select the Species checkbox for the species for which to specify the flux, and enter a value or expression for the inward flux in the corresponding field. Use a minus sign when specifying a flux directed out of the system. To use another boundary condition for a specific species, click to clear the checkbox for that species.

External convection

Set **Flux type** to **External convection** to prescribe a flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$J_0 = k_{\mathrm{c}}(c_{\mathrm{b}} - c)$$

where k_{c} is a mass transfer coefficient and c_{b} is the bulk concentration, the typical concentration far into the surrounding exterior domain.

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric, that is, where there is no mass flux across the boundary.

This boundary condition is identical to that of the No Flux node.

Flux Discontinuity

This node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n} \cdot [(\mathbf{J} + \mathbf{u}c)_{\mathrm{u}} - (\mathbf{J} + \mathbf{u}c)_{\mathrm{d}}] = N_0 \qquad \mathbf{J} = -D\nabla c$$

where the value N_0 (SI unit: mol/(m^2·s)) specifies the jump in total flux at the boundary. This can be used to model a boundary source, for example a surface reaction, adsorption, or desorption.

FLUX DISCONTINUITY

In this section the jump in species flux (or surface source) is specified.

Select the Species checkbox for the species to specify and enter a value or expression for the material flux jump in the corresponding field. To use a different boundary condition for a specific species, click to clear the checkbox for the flux discontinuity of that species.

Partition Condition

The **Partition Condition** node can be used to prescribe the relation between the concentration of a solute species in two adjoining immiscible phases. It can for example be used on interior boundaries separating two liquid phases, a gas-liquid interface, or on a boundary separating a liquid phase and a solid or porous media.

Select **Partition coefficient** from the **Relation** list to prescribe a linear relationship between the concentration on either side of a boundary. For a species concentration c_i, the ratio between the concentration on the upside and on the downside of the boundary ($c_{i,\mathrm{u}}$ and $c_{i,\mathrm{d}}$ respectively) is then defined in terms of a partition coefficient K_i in the manner of

$$K_i = \frac{c_{i,\,\mathrm{u}}}{c_{i,\,\mathrm{d}}}$$

Use the associated input field to prescribe the partition coefficient for each species.

Select **User defined** from the **Relation** list to set up a nonlinear relation between the up and downside concentrations. For such relations $f(c_i)_u = f(c_i)_d$, where $f(c_i)_u$ is the expression enforced on the upside. Use the associated input fields to enter the upside and downside expressions for each species.

The up and downside of the selected boundary is indicated with a red arrow in the Graphics window. The arrow points from the downside into the upside. Select the **Reverse direction** checkbox to reverse the direction of the arrow on the selected boundary, and update the definition of the up and downside concentrations accordingly.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

FURTHER READING

For an example of using a partition condition, see this application example:

Separation Through Dialysis: Application Library path **Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis**

Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the mass transport between two sets of boundaries. The node prescribes continuity in the concentration and the mass flux between the "source" and the "destination" side, respectively. Note that these names are arbitrary and does not influence the direction in which mass is transported. It is dictated by mass transfer equations in the adjacent domains.

BOUNDARY SELECTION

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

DESTINATION SELECTION

For more complex geometries, it might be necessary to specify the destination selection manually. To do so, right-click the **Periodic Condition** node and choose **Manual**

Destination Selection. You can then specify the boundaries that constitute the destination surfaces in the **Destination Selection** section.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. This section contains settings for specifying the type of constraint and whether to use a pointwise or weak constraint. See Constraint Settings for more information.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see Orientation of Source and Destination.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see Orientation of Source and Destination.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping Between Source and Destination** section, see Mapping Between Source and Destination.

FURTHER READING

For an example of using a periodic condition, see this application example:

	The KdV Equation and Solitons: Application Library path **COMSOL_Multiphysics/Equation_Based/kdv_equation**

Line Mass Source

The **Line Mass Source** feature models mass flow originating from a tube or line region with an infinitely small radius.

> This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the symmetry axis and the symmetry axis
3D	Edges

SPECIES SOURCE

Enter the source strength, $\dot{q}_{\mathrm{l,c}}$, for each species (SI unit: mol/(m·s)). A positive value results in species injection from the line into the computational domain, and a negative value means that the species is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Point Mass Source

The **Point Mass Source** feature models mass flow originating from an infinitely small domain around a point.

> This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SPECIES SOURCE

Enter the source strength, $\dot{q}_{p,c}$, for each species (SI unit: mol/s). A positive value results in species injection from the point into the computational domain, and a negative value means that the species is removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Open Boundary

Use this node to set up mass transport across boundaries where both convective inflow and outflow can occur. On the parts of the boundary where fluid flows into the domain, an exterior species concentration is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Transport of Diluted Species interface.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EXTERIOR CONCENTRATION

Enter a value or expression for the **Exterior concentration**.

Thin Diffusion Barrier

Use this boundary condition to model a thin layer through which mass is transported by diffusion only. The node is applicable on interior boundaries and can be used to avoid meshing thin structures.

THIN DIFFUSION BARRIER

Specify the **Layer thickness**, d_s, and input a **Diffusion coefficient**, $D_{s,c}$, for each of the species included.

Thin Impermeable Barrier

This feature models a thin mass transfer barrier. It is available on interior boundaries and introduces a discontinuity in the concentration across the boundary. On each side, a no-flux condition is prescribed for the mass transport implying that it acts as a barrier. The feature can be used to avoid meshing thin structures.

Solving a model involving coupled fluid flow and mass transfer, the Thin Impermeable Barrier feature can be combined with an Interior Wall feature in order to model a thin solid wall.

Equilibrium Reaction

Use this node to model a reaction where the kinetics is so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the reaction rate R_{eq}) to fulfill the equilibrium condition at all times in all space coordinates.

If the **Apply equilibrium condition on inflow boundaries** checkbox is selected, the specified inflow concentration values in all active **Inflow** boundary nodes for the physics interface are modified to comply with the equilibrium condition.

- A necessary requirement for this is feature to be available is that two or more species are solved for by the interface.
- This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EQUILIBRIUM CONDITION

The list defaults to **Equilibrium constant** or select **User defined**. For either option, the **Apply equilibrium condition on inflow boundaries** checkbox is selected by default.

For **Equilibrium constant**, enter an **Equilibrium constant** K_{eq} (dimensionless). Also enter a value or expression for the **Unit activity concentration** C_{a0} (SI unit: mol/m^3).

Selecting **Equilibrium constant** defines an equilibrium condition based on the stoichiometric coefficients, the species activities, and the law of mass action.

For **User defined**, enter an **Equilibrium expression** E_{eq} (dimensionless).

STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient ν_c (dimensionless). The default is 0. Use negative values for reactants and positive values for products in the modeled reaction.

Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium Reaction** node.

Surface Reactions

The **Surface Reactions** node can be used to account for the species boundary flux due to chemical reactions occurring on a surface (heterogeneous reactions). For a domain species participating in a surface reaction, the boundary flux corresponds to the reaction rate at the surface.

SURFACE REACTION RATE

Specify the surface reaction rate J_0 of each species resulting from the reactions. Note that if you have the Chemistry interface available, provided with the Chemical Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down list.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

FURTHER READING

For an example of using the Surface Reactions node, see this application example:

	Chemical Vapor Deposition of GaAs: Application Library path **Chemical_Reaction_Engineering_Module/ Reactors_with_Mass_and_Heat_Transfer/gaas_cvd**

Surface Equilibrium Reaction

Use this node to model an equilibrium reaction on a boundary (surface). The settings for this node are similar to Equilibrium Reaction. Note that a necessary requirement

for this is feature to be available is that two or more species are solved for by the interface.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Fast Irreversible Surface Reaction

This boundary node defines an irreversible reaction where the kinetics is so fast that the only factor limiting the reaction rate is the transport of a species to the reacting surface.

The node will set the **Rate limiting species concentration to zero** at the boundary, and balance the fluxes of the species participating in the reaction and the current densities according to the Stoichiometric Coefficients settings.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Electrode Coupling

Use this node to add a molar source in a domain that is coupled to one or multiple Porous Electrode Reaction nodes of an Electrochemistry Interface.

The molar source is calculated from the number of electrons, stoichiometric coefficients, and volumetric current densities of the coupled porous electrode reactions specified in the **Reaction Coefficients** subnodes.

In the Transport of Concentrated Species interface, the molar sources (or sinks) are multiplied by the species molar masses to obtain the corresponding mass sources.

Additional Reaction Coefficients subnodes are available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass source or sink, which is often the case in gas diffusion electrodes, you need to also add a corresponding mass source/sink in the Fluid Flow interface. (A **Reacting Flow** multiphysics node adds the associated source/sink term in a Fluid Flow interface automatically.)

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Reaction Coefficients

Add this node to the Electrode Surface Coupling and Porous Electrode Coupling features to define molar fluxes and sources based on electrode current densities in an **Electrochemistry** interface.

The molar flux or source is proportional to the stoichiometric coefficients and the current density according to Faraday's law.

Current densities from **Electrode Reaction** (i_{loc}, SI unit: A/m^2) or **Porous Electrode Reaction** nodes (i_{v}, SI unit: A/m^3) of any **Electrochemistry** interface in the model are available for selection as the **Coupled reaction**, and user-defined expressions are also supported.

Enter the **Number of participating electrons** n_m (dimensionless) and the **Stoichiometric coefficient** v_c (dimensionless) as explained in the theory section linked below.

Use multiple subnodes to couple to multiple reactions.

Electrode Surface Coupling

Use this node to define a flux boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flux is proportional to the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficients subnodes.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass flux over the boundary, which is often the case for gas diffusion electrodes, you need to also add a corresponding Electrode Surface Coupling node in the Fluid Flow interface.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Species transport through a porous medium is affected both by properties of the fluid phase, and as well as properties of the solid matrix. These properties are defined in the Fluid (Porous Medium) and Porous Matrix subnodes respectively. The Porous Medium node supports material properties using a Porous Material node, where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the **Porous Medium** to account for the corresponding transport mechanism.

Fluid (Porous Medium)

Use this node to specify the mass transfer in the mobile fluid solvent filling the pores of a porous medium. It is used as a subnode to Porous Medium.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat

Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Fluid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Fluid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Fluid diffusion coefficient** list.

For **User defined**, enter a value or expression for the **Fluid diffusion coefficient** $D_{\mathrm{F,i}}$ of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an **Effective diffusivity model** to account for the reduced diffusivity. The available models are **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **No correction**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{\mathrm{F,i}}$ (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products.For details, see https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected. From the **Electric potential** list, select the source of the electric field.

- For **User defined**, enter a value or expression for the **Electric potential** V. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value or expression of the effective mobility $u_{\mathrm{me,i}}$.

Enter the **Charge number** z_{c} for each species.

Porous Matrix

This node sets the porosity when modeling transport of diluted species in a Porous Medium or an Unsaturated Porous Medium. The porosity corresponds to the volume fraction occupied by the species containing fluid.

- By default the porosity of the solid matrix, ε_{p}, is taken **From material**. The **Porous Matrix** node supports the use of a **Porous Material** added to the Materials branch. In this case the porosity is defined in the manner of

$$\varepsilon_{\mathrm{p}} = 1 - \sum_{i} \theta_{\mathrm{s},\,i} - \sum_{i} \theta_{\mathrm{imf},\,i}$$

  where $\theta_{\mathrm{s},i}$ and $\theta_{\mathrm{imf},i}$ are the volume fractions given in **Solid** and **Immobile Fluids** subnodes under the **Porous Material** node.
- Select **From pellet bed densities** to compute the porosity using the (dry bulk) **Bed density** ρ_{b} and the (single phase) **Pellet density** ρ_{pe}. The porosity is then defined from

$$\varepsilon_p = 1 - \frac{\rho_b}{\rho_{pe}}$$

- For **User defined**, enter a value or expression for the porosity.

Dispersion

Local variations in the velocity as the fluid flows around solid particles lead to mechanical mixing, referred to as dispersion. Use this feature to account for dispersion in a Porous Medium or a Unsaturated Porous Medium

This subfeature is available when both the **Mass transfer in porous media mass transfer** checkbox and the **Convection** checkbox are selected in the **Settings** window for the physics interface.

Select the **Specify dispersion for each species individually** checkbox to specify the dispersion tensor D_D (SI unit: m^2/s) for each species separately. When not selected the same dispersion tensor D_D is used for all species.

Select an option from the **Dispersion tensor** list — **Dispersivity** or **User defined**.

Select **Dispersivity** to specify the dispersion in terms of dispersivities (SI unit: m). Select an option from the **Dispersivity model** list: **Isotropic** (the default) or **Transverse isotropic** based on the properties of the porous media. For isotropic porous media, specify the longitudinal and transverse dispersivities. For transverse isotropic porous media, specify the longitudinal, horizontal transverse, and vertical transverse dispersivities.

For **User defined**, specify the dispersion components in terms of constants or expressions. Select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** to enable the appropriate tensor components.

Unsaturated Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

Use this node to model the concentration of diluted species transported by a liquid (mobile fluid phase) in a partially filled solid porous medium. The interstices of the porous medium contains the liquid carrier phase and gas pockets. Apart from

convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and volatilization.

!	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The properties of each phase present are defined using the Liquid, the Gas, and the Porous Matrix subnodes respectively. The Unsaturated Porous Medium node supports material properties using a Porous Material node, where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the **Unsaturated Porous Medium** to account for the corresponding transport mechanism.

Liquid

Use this node to specify the mass transfer in the mobile liquid solvent present in the pores of the Unsaturated Porous Medium.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

SATURATION

Select **Saturation** or **Liquid volume fraction** from the list.

For **Saturation**, enter a value for s (dimensionless) between 0 and 1. The liquid volume fraction is then computed from the saturation and porosity as $\theta_l = \varepsilon_p s$.

For **Liquid volume fraction**, enter a value for θ_l (dimensionless) between 0 and the value of the porosity.

Select a **Liquid fraction time change**: **Liquid fraction constant in time** (the default), **Time change in liquid fraction**, or **Time change in pressure head**.

- For **Time change in fluid fraction**, enter $\mathrm{d}\theta/\mathrm{d}t$ (SI unit: $1/\mathrm{s}$).
- For **Time change in pressure head**, enter $\mathrm{d}H_\mathrm{p}/\mathrm{d}t$ (SI unit: m/s) and a **Specific moisture capacity** C_m (SI unit: $1/\mathrm{m}$). If a Darcy's Law interface is included in the component, the time change in pressure head solved for can be selected.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent liquid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Liquid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Liquid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Liquid diffusion coefficient** list.

For **User defined**, enter a value or expression for the **Liquid diffusion coefficient** $D_{\mathrm{L},i}$ of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an **Effective diffusivity model, liquid** to account for the reduced diffusivity in the liquid. The available models are **Millington and Quirk model**

(the default), **Bruggeman model**, **Tortuosity model**, or **No correction**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{L,i}$ (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. For details see: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected. From the **Electric potential** list, select the source of the electric field.

- For **User defined**, enter a value or expression for the **Electric potential** V. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value or expression of the effective mobility $u_{me,i}$.

Enter the **Charge number** z_c for each species.

Gas

Use this node to specify the mass transfer in the gas phase present in the pores of the Unsaturated Porous Medium.

DIFFUSION

The settings for the diffusion of each species in the gas phase are identical to those in the Liquid subnode.

VOLATILIZATION

Enter a value for the volatilization isotherm $k_{G,c}$ (dimensionless) for each species.

Adsorption

Use this node to model adsorption of the (fluid phase) solute species onto the surface of the porous matrix. It is available as a subnode to the Porous Medium and the Unsaturated Porous Medium nodes.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

MATRIX PROPERTIES

The density of the porous media is needed when modeling adsorption to the surface of the porous matrix. Choose to input either the **Dry bulk density** ρ, or the **Solid phase density** ρ_s. The former is the density of the porous matrix including empty pores, while the latter corresponds to the density of the pure solid phase. The density can be defined from the domain material by selecting **From material**, or from a user defined expression. When a **Porous Material** is used on the selection, the density will be requested from a **Solid** subfeature. Several **Solid** features can be used to model a homogeneous mixture of several solid components.

ADSORPTION

Select an **Adsorption isotherm** — **Langmuir**, **Freundlich**, **Toth**, **BET**, or **User defined** to specify how to compute c_P, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

- For **Langmuir**:

$$c_P = c_{P\max}\frac{K_L c}{1+K_L c} \quad , \quad K_P = \frac{\partial c_P}{\partial c} = \frac{K_L c_{P\max}}{(1+K_L c)^2}$$

  Enter a **Langmuir constant** $k_{L,c}$ (SI unit: m^3/mol) and an **Adsorption maximum** $c_{p,max,c}$ (SI unit: mol/kg).

- For **Freundlich**:

$$c_P = K_F\left(\frac{c}{c_{ref}}\right)^N \quad , \quad K_P = \frac{\partial c_P}{\partial c} = N\frac{c_P}{c}$$

Enter a **Freundlich constant** $k_{F,c}$ (SI unit: mol/kg), a **Freundlich exponent** $N_{F,c}$ (dimensionless), and a **Reference concentration** $c_{ref,c}$ (SI unit: mol/m^3).

- For **Toth**:

$$c_P = c_{Pmax}\frac{b_T c}{(1+(b_T c)^{N_T})^{1/N_T}}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = c_{Pmax} b_T (1+(b_T c)^{N_T})^{-\left(1+\frac{1}{N_T}\right)}$$

Enter a **Toth constant** $b_{T,c}$ (SI unit: m^3/mol), a **Toth exponent** $N_{T,c}$ (dimensionless), and an **Adsorption maximum** $c_{p,max,c}$ (SI unit: mol/kg).

- For **BET (Brunauer-Emmett-Teller)**:

$$c_P = \frac{K_B c_0 c}{(c_S - c)\left(1+(K_B-1)\frac{c}{c_S}\right)}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = \frac{K_B c_0 c_S((K_B-1)c^2 + c_S^2)}{(c-c_S)^2(c_S+(K_B-1)c)^2}$$

Enter a **BET constant** $K_{B,c}$ (dimensionless), a **Monolayer adsorption capacity** $c_{0,c}$ (SI unit: mol/kg), and an **Saturation concentration** $c_{S,c}$ (SI unit: mol/m^3).

- For **User defined** enter an **Adsorption isotherm** $c_{P,c}$ (SI unit: mol/kg):

$$c_P = f(c)$$

For more information, see in the theory section.

FURTHER READING

See the theory chapter in the section .

Volatilization

This feature is available when the **Mass transfer in porous media** checkbox is selected in the **Settings** window for the physics interface.

Use this feature to model mass transfer at the boundary due to volatilization. The species dissolved in the liquid are assumed to be vaporized at the boundary, and transported into the surrounding bulk region due to convection and diffusion. The mass transfer at the boundary is defined as

$$-\mathbf{n}\cdot\mathbf{J}_c = -h_c(k_{G,c}c - c_{Gatm,c})$$

where h_c is the mass transfer coefficient, $k_{G,c}$ the volatilization coefficient, and $c_{Gatm,c}$ the concentration in the surrounding atmosphere.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

VOLATILIZATION

Enter a **Mass transfer coefficient** h_c defining the transfer into the surrounding media. This can be given by boundary layer theory. When assuming that no convective flow is present in the surrounding, the mass transfer coefficient can be defined from the gas diffusion coefficient D_{Gc} and the thickness of the diffusion layer d_s in the manner of

$$h_c = \frac{D_{Gc}}{d_s}$$

Also give the atmospheric concentration for each species, $c_{Gatm,c}$. The **Volatilization** coefficient $k_{G,c}$ for each species are taken from the adjacent Unsaturated Porous Medium domain.

Species Source

In order to account for consumption or production of species in porous domains, the **Species Source** node adds source terms expressions S_i to the right-hand side of the species transport equations.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

If there are several types of domains, with subsequent and different reactions occurring within them, it might be necessary to remove some domains from the selection. These are then defined in an additional **Species Source** node.

SPECIES SOURCE

Add a source term S_i (SI unit: mol/(m^3·s)) for each of the species solved for. Enter a value or expression in the field of the corresponding species.

Hygroscopic Swelling

The **Hygroscopic Swelling** multiphysics coupling node ( ) is used for moisture concentration coupling between the Solid Mechanics interface and either the Transport of Diluted Species or Transport of Diluted Species in Porous Media interfaces.

Hygroscopic swelling is an effect of internal strain caused by changes in moisture content. This volumetric strain can be written as

$$\varepsilon_{hs} = \beta_h M_m (c_{mo} - c_{mo,ref})$$

where β_h is the coefficient of hygroscopic swelling, M_m is the molar mass, c_{mo} is the moisture concentration, and $c_{mo,ref}$ is the strain-free reference concentration.

This feature requires a license of either the MEMS Module or the Structural Mechanics Module. The multiphysics feature will appear automatically if both the Transport of Diluted Species and the Solid Mechanics interfaces are added to the same component. For the most current information about licensing, please see https://www.comsol.com/products/specifications/.

FURTHER READING

More information about how to use hygroscopic swelling can be found in the Hygroscopic Swelling section in the *Structural Mechanics Module User's Guide*.

More information about multiphysics coupling nodes can be found in the section The Multiphysics Branch.

Out-of-Plane Flux

The out-of-plane flux node is used to prescribe a flux in an out-of-plane domain, and it can be used to reduce a model geometry to 2D, or even 1D, when the concentration variation is small in one or more directions. This could be the case for example when the object to model is thin or slender. Figure 8-1 shows examples of possible situations in which this type of geometry reduction can be applied.

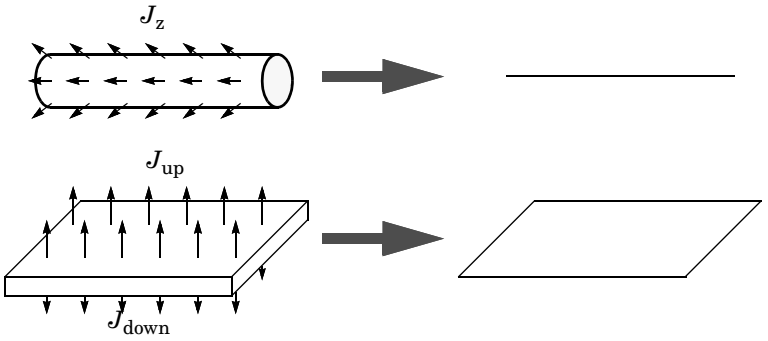

Figure 8-1: Geometry reduction from 3D to 1D (top) and from 3D to 2D (bottom).

For a 1D component this node adds a single out-of-plane molar flux $J_{0,z,i}$ for species i. For a 2D component two fluxes can be prescribed for each species; $J_{0,u,i}$ for the upside of the domain, and $J_{0,d,i}$ for the downside of the domain.

The fluxes are added as a source contribution to the right-hand side of the transport equation. For example, in 2D components with diffusion, convection, and out-of-plane flux present, the mass transfer of species i is defined by the mass conservation equation

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i + S_{\mathrm{opf},i}, \tag{8-1}$$

where $S_{\mathrm{opf},i}$ is the out-of-plane source for species i

$$S_{\mathrm{opf},i} = \frac{J_{0,i}}{d_z} = \frac{J_{0,u,i} + J_{0,d,i}}{d_z}.$$

For external convection on the upside and the downside of the domain, the out-of-plane flux is

$$J_{0,i} = k_{\mathrm{c,u},i}(c_{\mathrm{b,u},i} - c_i) + k_{\mathrm{c,d},i}(c_{\mathrm{b,d},i} - c_i)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain. The prescribed flux, J_0, can include any arbitrary user-specified expressions. It can be a constant or a function of a dependent variable or independent variables.

UPSIDE INWARD FLUX

For 1D components, enter the **cross-sectional perimeter** P_c to get the out-of-plane flux

$$J_{0,i} = P_c J_{0,\mathrm{z},i}.$$

The default value of P_c is the circumference. Either keep the default value, for a circular cross-section shape, or edit the value to get a user-defined shape of the out-of-plane cross-section.

The available flux type options are **General inward flux** and **External convection**. Select the **Species** checkbox for the species for which to specify the flux, and enter a value or expression for the inward flux in the corresponding field. Use a minus sign when specifying a flux directed out of the system. To use another boundary condition for a specific species, click to clear the checkbox for that species.

Set **Flux type** to **External convection** to prescribe a flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$J_0 = k_c(c_b - c)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain.

DOWNSIDE INWARD FLUX

The available options are **General inward flux** and **External convection**. The settings are the same as for the Upside Inward Flux section.

FURTHER READING

For an example of using the Out-of-Plane Flux node, see this application example:

Cross-Flow Mass Transfer in a Thin Domain: Application Library path **Chemical_Reaction_Engineering_Module/Tutorials/thin_domain**

Fracture

Use this node to model mass transport along thin fractures in porous media. The node assumes that the transport in the tangential direction along the fracture is dominant as a result of lower flow resistance.

The Fracture feature has two default subfeatures — the Fluid (Fracture) subfeature where convection and diffusion are specified and the Fracture Material subfeature where the porosity ε_p is defined.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

FRACTURE PROPERTIES

Specify a value for the **Fracture thickness** d_{fr}.

For the **Fracture** boundary condition, there are a number of **Attributes** available which can be accessed either via the **Physics** Ribbon toolbar (for Windows) or by right-clicking on the **Fracture** node. These attributes are identical to the Boundary, Edge, Point, and Pair Nodes for the Transport of Diluted Species in Fractures Interface described, for example, in the *Chemical Reaction Engineering Module User's Guide*.

Fluid (Fracture)

Use this node to specify the mass transfer in the mobile fluid solvent filling the pores of a fracture.

It uses the same input options as the Fluid (Porous Medium) subfeature under the Porous Medium feature. There are further details about the settings.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from **Default Model Inputs** under **Global Definitions** or by a locally defined **Model Input**. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use a Fracture feature in a Darcy's Law interface to compute the fluid flow velocity in the fracture.

For **User defined**, enter values or expressions for the velocity components in the table shown

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

The **Diffusion** settings are similar to those for the diffusion coefficients in the Fluid (Porous Medium) node under Porous Medium.

Fracture Material

Specify the **Porosity** ε_p (dimensionless) of the porous matrix. This is by default taken **From material**. Select **From pellet bed densities** to compute the porosity from the (dry bulk) **Bed density** ρ_b and the (single phase) **Pellet density** ρ_{pe} through the relation

$$\varepsilon_p = 1 - \frac{\rho_b}{\rho_{pe}}$$

For **User defined**, enter a value or expression for the porosity.

The Transport of Concentrated Species Interface

The **Transport of Concentrated Species (tcs)** interface ( ), found under the **Chemical Species Transport** branch ( ) when adding a physics interface, is used to study gaseous and liquid mixtures where the species concentrations are of the same order of magnitude and none of the species can be identified as a solvent. In this case, properties of the mixture depend on the composition, and the molecular and ionic interactions between all species need to be considered. The physics interface includes models for multicomponent diffusion, where the diffusive driving force of each species depends on the mixture composition, temperature, and pressure.

The physics interface solves for the mass fractions of all participating species. Transport through convection, diffusion, and migration in an electric field can be included.

It supports simulations of transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The physics interface defines the equations for the species mass fractions, including a diffusion model (Mixture-averaged, Maxwell–Stefan, or Fick's law).

The available transport mechanisms and diffusion models differs between various COMSOL products (see https://www.comsol.com/products/specifications/).

Some examples of what can be studied with this physics interface include:

- The evolution of a chemical species transported by convection and diffusion.
- The migration in an electric field in the case of ionic species, in mixtures and solutions that cannot be deemed as being diluted.
- Concentrated solutions or gas mixtures, where the concentration of all participating species are of the same order of magnitude, and their molecular and ionic interaction with each other therefore must be considered. This implies that the diffusive transport of a single species is dependent on the mixture composition, and possibly on the temperature, the electric potential, the pressure, or any combination.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **No Flux**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and reactions. You can also right-click **Transport of Concentrated Species** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tcs`.

EQUATION

The basic equation for the conservation of mass of a species i is:

$$\frac{\partial}{\partial t}(\rho\omega_i) + \nabla \cdot (\rho\omega_i \mathbf{u}) = -\nabla \cdot \mathbf{j}_i + R_i \tag{8-2}$$

Using the continuity equation, the sum of all species equations, the equation can be recast in its nonconservative form:

$$\rho\frac{\partial}{\partial t}(\omega_i) + \rho(\mathbf{u} \cdot \nabla)\omega_i = -\nabla \cdot \mathbf{j}_i + R_i \tag{8-3}$$

This form of the equation is the one used in the Transport of Concentrated Species interface. The equation displayed in the interface changes depending on the active transport mechanisms, the selected diffusion model, and the type of reactions modeled.

OUT-OF-PLANE THICKNESS

For 2D components, the **Thickness** field (default value: 1 m) defines a parameter for the thickness of the geometry perpendicular to the two-dimensional cross-section. Both constant and varying thicknesses are supported. The value of this parameter is used, among other things, to automatically calculate mass flow rates from the total mass flux.

CROSS-SECTIONAL AREA

For 1D components, enter a **Cross-sectional area** A_c (SI unit: m^2) to define a parameter for the area of the geometry perpendicular to the 1D component. Both constant and varying areas are supported.The value of this parameter is used, among other things, to automatically calculate mass flow rates from the total mass flux. The default is 1 m^2.

TRANSPORT MECHANISMS

The Transport of Concentrated Species interface always accounts for transport due to convection and diffusion.

The available diffusion models and the additional transport mechanisms differs between various COMSOL products (see https://www.comsol.com/products/specifications/).

Diffusion Model

- The **Maxwell–Stefan** option employs the most detailed diffusion model, but is also the most computationally expensive. The model is intended for diffusion dominated models, and requires that the multicomponent Maxwell–Stefan diffusivities of all component pairs are known.
- The **Mixture-averaged** option is less computationally expensive than the Maxwell–Stefan model. It is a simpler model that can be used when variations in the partial pressures and temperature can be assumed to not affect the multicomponent diffusion. The model includes stabilization but requires the multicomponent Maxwell–Stefan diffusivities of all component pairs.
- The **Fick's law** model is a general model that should be used when the diffusion is assumed Fickian, or when no multicomponent diffusivities are available. Also, when molecular diffusion is not the dominating transport mechanism and a robust but low order model is wanted, the Fick's law options should be used. The model includes stabilization.

Additional Transport Mechanisms

Under **Additional transport mechanisms**, click to select or clear any combination of checkboxes as needed.

Migration in Electric Field

Select the **Migration in electric field** checkbox to activate migration of ionic species due to an electric field. The resulting migration term is part of the relative mass flux vector.

Mass Transport in Porous Media

The **Mass transport in porous media** checkbox activates functionality specific to species transport in porous media. When selected the following domain features are enabled:

- Porous Medium
- Porous Electrode Coupling

Maxwell–Stefan Diffusion Model

When using the **Maxwell–Stefan** diffusion model the relative mass flux vector is

$$\mathbf{j}_i = -\rho\omega_i \sum_{k=1}^{Q} D_{ik}\mathbf{d}_k - \frac{D_i^T}{T}\nabla T$$

where $\tilde{D}_{ik}$ (SI unit: m^2/s) are the multicomponent Fick diffusivities, $\mathbf{d}_k$ (SI unit: 1/m) is the diffusional driving force, T (SI unit: K) is the temperature, and D_i^T (SI unit: kg/(m·s)) is the thermal diffusion coefficient.

The diffusional driving force is defined as

$$\mathbf{d}_k = \nabla x_k + \frac{1}{p}\left[(x_k - \omega_k)\nabla p - \rho\omega_k\mathbf{g}_k + \omega_k \sum_{l=1}^{Q} \rho\omega_l\mathbf{g}_l\right] \tag{8-4}$$

where $\mathbf{g}_k$ is an external force (per unit mass) acting on species k. In the case of an ionic species, the external force due to the electric field, which is added by selecting the **Migration in electric field** checkbox, is

$$\mathbf{g}_k = -\frac{z_k F}{M_k}\nabla\phi \tag{8-5}$$

where z_k is the species charge number, F (SI unit: A·s/mol) is Faraday's constant and ϕ (SI unit: V) is the electric potential.

Mixture-Averaged Diffusion Model

When using the **Mixture-averaged** diffusion model, the diffusive flux is formulated in terms of a mixture-averaged diffusion coefficient representing the diffusion of each species into the resulting mixture. The diffusion coefficient is based on the multicomponent Maxwell–Stefan diffusivities D_{ik}. The **Mixture-averaged** diffusion model is computationally less expensive, and significantly more robust than the Maxwell–Stefan Diffusion Model, but constitutes an approximation of the multicomponent flux. For information on the flux formulation in this case see Multicomponent Diffusion: Mixture-Averaged Approximation.

Fick's Law Diffusion Model

When using the **Fick's law** diffusion model, the diffusive flux is formulated in terms of a Fickian diffusion coefficient. The **Fick's law** diffusion model is computationally less expensive and significantly more robust than the Maxwell–Stefan Diffusion Model, but constitutes an approximation of the multicomponent flux. For information on the flux formulation in this case see Multispecies Diffusion: Fick's Law Approximation.

SPECIES

Select the species that this physics interface solves for using the mass constraint in Equation 8-6 (that is, its value comes from the fact that the sum of all mass fractions must equal 1). In the **From mass constraint** list, select the preferred species. To minimize the impact of any numerical and model introduced errors, use the species with the highest concentration. By default, the first species is used.

$$\omega_1 = 1 - \sum_{i=2}^{Q} \omega_i \tag{8-6}$$

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**.

- Two consistent stabilization methods are available — **Streamline diffusion** and **Crosswind diffusion**. Both are active by default.

  The **Residual** setting applies to both the consistent stabilization methods. **Approximate residual** is the default setting and it means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and computationally faster. If required, select **Full residual** instead.

- There is one inconsistent stabilization method, **Isotropic diffusion**, which is available when using the Mixture-Averaged Diffusion Model or Fick's Law Diffusion Model.

ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Regularization

From the **Regularization** list, select **On** (the default) or **Off**. When turned **On**, regularized mass fractions are calculated such that

$$0 \le w_{i,\,\mathrm{reg}} \le 1$$

Regularized mass fractions are used for the calculation of composition-dependent material properties, such as the density.

Diffusion

The **Diffusion** settings are available for the approximate diffusion models Mixture-averaged and Fick's law.

When the **Mixture diffusion correction** is enabled, a flux correction is added to ensure that the net diffusive flux is zero. This typically also mean that the solution becomes less sensitive to the species selected to be computed from the mass constraint in the Species section. More information on this correction is available in the theory section Multicomponent Diffusion: Mixture-Averaged Approximation.

The **Diffusion flux type** list controls the whether the molecular flux is assumed proportional to the mole fraction or the mass fraction. See Multicomponent Diffusion: Mixture-Averaged Approximation or Multispecies Diffusion: Fick's Law Approximation for information on the diffusive flux formulation.

Pseudo Time Stepping

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary** equation form is used in order to speed up convergence. When selected, a CFL number expression should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator. For more information, see Pseudo Time Stepping for Mass Transport.

DISCRETIZATION

To display all settings available in this section, click the **Show** button ( ) and select **Advanced Physics Options**.

For more information about these settings, see the *Discretization* section under The Transport of Diluted Species Interface.

	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

	• Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface • Theory for the Transport of Concentrated Species Interface

- *Species Transport in the Gas Diffusion Layers of a PEM*: Application Library path **Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pem_gdl_species_transport_2d**

  Web link: https://www.comsol.com/model/species-transport-in-the-gas-diffusion-layers-of-a-pem-260

DEPENDENT VARIABLES

Add or remove species in the model and also change the names of the dependent variables that represent the species concentrations.

Specify the **Number of species**. There must be at least two species. To add a single species, click the **Add concentration** button (+) under the table. To remove a species, select it in the list and click the **Remove concentration** button ( ) under the table. Edit the names of the species directly in the table.

The species are dependent variables, and their names must be unique with respect to all other dependent variables in the component.

Adding a Chemical Species Transport Interface

The Transport of Concentrated Species in Porous Media Interface

This interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the chemical composition in a fluid mixture transported through the interstices of a porous media. The interface is the same as the *Transport of Concentrated Species* interface but it has a Porous Medium node added by default. All other features for porous media transport is always available.

This interface is dedicated to analyzing mass transport in porous media where the chemical species may be subjected to convection, diffusion, and migration in an electric field. The interface also includes reaction rate expressions and source terms for modeling chemical reactions in porous media. It is also possible to include regions with free flow.

The main feature of the interface is the **Porous Medium** node which adds the governing equations for the mass fractions of all present species. It has two subnodes, **Fluid** and

Porous Matrix, which in turn are used to define the physical properties corresponding to each phase, and to prescribe the transport properties. The latter are typically the flow field, and when applicable, the electric field. The **Porous Medium** node supports the use of a Porous Material for defining phase-specific properties, and for sharing them among different physics interfaces.

When this physics interface is added, the following default nodes are also added to the **Model Builder** — **Porous Medium**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, reaction rate expressions, and species sources. You can also right-click **Transport of Concentrated Species in Porous Media** to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as The Transport of Concentrated Species Interface.

Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface

The Transport of Concentrated Species Interface has these domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

	In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.

These nodes are described in this section or as indicated:

- Electrode Surface Coupling
- Equilibrium Reaction
- Fluid (Porous Medium)
- Flux
- Flux Discontinuity
- Inflow
- Initial Values
- Mass Fraction
- No Flux
- Open Boundary
- Out-of-Plane Flux
- Outflow
- Porous Matrix
- Porous Medium
- Reaction
- Reaction Sources
- Species Properties
- Surface Equilibrium Reaction
- Symmetry
- Thin Impermeable Barrier[1]
- Fluid

Some features require certain add-on modules. See details https://www.comsol.com/products/specifications/

[1] The node is described for the Transport of Diluted Species interface.

Prescribing Conditions on Fluid-Solid Interfaces

Defining conditions on interfaces between different phases, typically a wall in contact with a fluid, it is worthwhile to be careful with how variables in the conditions are evaluated. COMSOL Multiphysics supports that variables are defined differently on adjacent domains (or any other geometry dimension). Evaluating a variable with differing definitions, the mean value is returned on a boundary separating the different domains. The density, pressure, or temperature are examples of variables that may differ in a fluid and a solid. In order to specify on which side a variable is evaluated, the up and down operators (described in the *COMSOL Multiphysics Reference Manual*) can be used.

Species Properties

Use this node to define parameters specific to each of the species.

The node will change its label depending on what inputs are available in the node. If only **Molar Mass** is available, it will be labeled “Species Molar Masses”.

MOLAR MASS

Enter a value or expression for the **Molar mass** M_w for each species. The default value is 0.032 kg/mol, which is the molar mass of O_2 gas.

CHARGE

This section is available when the **Migration in electric field** checkbox is selected in the Transport Mechanisms section of the interface. Enter the charge number z_w (dimensionless, but requires a plus or minus sign) for each species.

Fluid

The **Fluid** node is the main node used to model mass transfer in a fluid mixture with the Transport of Concentrates species interface. The node adds the equations governing the mass fractions of all present species, and provides inputs for the transport mechanisms and for the material properties of the fluid mixture.

The settings in this node are dependent on the checkboxes selected under Transport Mechanisms in the Settings window of the Transport of Concentrated Species interface.

The options available in this feature differs between COMSOL products. (See https://www.comsol.com/products/specifications/).

MODEL INPUTS

Specify the temperature and pressure to be used in the physics interface. The temperature model input is used when calculating the density from the ideal gas law, but also when thermal diffusion is accounted for by supplying thermal diffusion coefficients. The pressure model input is used in the diffusional driving force in Equation 8-4 (that is, when a Maxwell–Stefan Diffusion Model is used) and when calculating the density from the ideal gas law.

Temperature

Select the source of the **Temperature** field T:

- Select **User defined** to enter a value or an expression for the temperature (SI unit: K). This input is always available.
- If required, select a temperature defined by a Heat Transfer interface present in the model (if any). For example, select **Temperature (ht)** to use the temperature defined by the Heat Transfer in Fluids interface with the `ht` name.

Absolute Pressure

Select the source of the **Absolute pressure** p:

- Select **User defined** to enter a value or an expression for the absolute pressure (SI unit: Pa). This input is always available.
- In addition, select a pressure defined by a Fluid Flow interface present in the model (if any). For example, select **Absolute pressure (spf)** to use the pressure defined in a Laminar Flow interface with `spf` as the name.

DENSITY

Define the density of the mixture and the molar masses of the participating species.

Mixture Density

Select a way to define the density from the **Mixture density** list — **Ideal gas** or **User defined**:

- For **Ideal gas**, the density is computed from the ideal gas law in the manner of:

$$\rho = \frac{pM}{R_g T}$$

  Here M is the mean molar mass of the mixture and R_g is the universal gas constant. The absolute pressure, p, and temperature, T, used corresponds to the ones defined in the Model Inputs section.
- For **User defined** enter a value or expression for the **Mixture density** ρ.

CONVECTION

Select the source of the **Velocity field** $\mathbf{u}$:

- Select **User defined** to enter manually defined values or expressions for the velocity components. This input is always available.
- Select a velocity field defined by a Fluid Flow interface present in the model (if any). For example, select **Velocity field (spf)** to use the velocity field defined by the **Fluid**

Properties node `fp1` in a Single-Phase Flow, Laminar Flow interface with `spf` as the Name.

DIFFUSION

Specify the molecular and thermal diffusivities of the present species based on the selected **Diffusion model**.

When using a Maxwell–Stefan Diffusion Model or a Mixture-Averaged Diffusion Model, select the **Binary diffusion input type** (Table or Matrix) and specify the **Maxwell–Stefan diffusivities** in the table or matrix, then enter the **Thermal diffusion coefficients** D_w^T.

When using a Fick's Law Diffusion Model, specify the **Diffusion coefficient** D_w^F and the **Thermal diffusion coefficients** D_w^T for each of the species.

Maxwell–Stefan Diffusivity Matrix

Using a Maxwell–Stefan Diffusion Model or a Mixture-Averaged Diffusion Model, the **Maxwell–Stefan diffusivity matrix** D_{ik} (SI unit: m^2/s) can be specified by a table or matrix. For a simulation involving Q species the Maxwell–Stefan diffusivity matrix is a Q-by-Q symmetric matrix, where the diagonal components are 1. Enter values for the upper triangular components, D_{ij}, which describe the interdiffusion between species i and j. For the table input type, only upper triangular components (D_{ij}) are listed. The name of species pair consists of species in the first and second column. For the matrix input type, the numbering of the species corresponds to the order, from top to bottom, used for all the input fields for species properties (see for example the molar mass fields in the Density section).

Diffusion Coefficient

Using a Fick's Law Diffusion Model, the diffusion is by default assumed to be isotropic and governed by one **Diffusion coefficient** D_w^F (SI unit: m^2/s) for each species. To allow for a general representation, it is also possible to use diffusion matrices (diagonal, symmetric, or anisotropic).

Thermal Diffusion Coefficient

To model thermal diffusion, prescribe the **Thermal diffusion coefficients** D_i^T (SI unit: kg/(m·s)), by entering one thermal diffusion coefficient for each species in the corresponding field. In a multicomponent mixture, the sum of the thermal diffusion coefficients is zero. The default value for all thermal diffusion coefficients is 0.

Specify the molecular and thermal diffusivities of the present species based on the selected **Diffusion model**.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected for the Transport of Concentrated Species interface.

Electric Potential

- Select **User defined** to enter a value or expression for the electric potential. This input is always available.
- If required, select an electric potential defined by an AC/DC interface that is present in the model (if any). For example, select **Electric potential (ec)** to use the electric field defined by the Current Conservation node `cucn1` in an Electric Currents interface `ec`.

Settings for the mobilities are used for the **Mixture-averaged** and **Fick's law** transport models. By default the mobility is set to be calculated based on the species diffusivities and the temperature using the **Nernst-Einstein relation**. To manually specify the mobilities, select **User defined** for the mobility $u_{\mathrm{m,c}}$ (SI unit: s·mol/kg) and enter one value for each species.

The temperature (if you are using mobilities based on the Nernst–Einstein relation) is taken from the **Model Inputs** section.

Porous Medium

Use this node to model the composition in a gas or liquid mixture as it is transported though the interstices of solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through reactions in the fluid phase.

Species transport in a porous medium is affected both by properties of the fluid phase as well as properties of the solid matrix. These properties are defined in the Fluid (Porous Medium) node and the Porous Matrix node respectively. The Porous Medium node supports material properties using a Porous Material node, where properties are defined per phase in a similar manner.

Fluid (Porous Medium)

Use this node to specify the mass transport in a fluid phase filling the pores of a porous medium. It is used as a subnode to Porous Medium.

MODEL INPUTS

Specify the temperature and pressure in the fluid. The temperature model input is used when calculating the density from the ideal gas law, but also when thermal diffusion is accounted for by supplying thermal diffusion coefficients. The pressure model input is used in the diffusional driving force in Equation 8-4 (that is, when a Maxwell–Stefan Diffusion Model is used) and when calculating the density from the ideal gas law.

Temperature

Select the source of the **Temperature** field T:

- Select **User defined** to enter a value or an expression for the temperature.
- When present, select a temperature defined by a Heat Transfer interface in the model. For example, select **Temperature (ht)** to use the temperature defined by the Heat Transfer in Fluids interface with the `ht` name.

Absolute Pressure

Select the source of the **Absolute pressure** p:

- Select **User defined** to enter a value or an expression for the absolute pressure.
- When present, select a pressure defined by a Fluid Flow interface present in the model. For example, select **Absolute pressure (spf)** to use the pressure defined in a Laminar Flow interface with `spf` as the name.

DENSITY

Use this section to define the density of the fluid phase, and to specify the molar masses of the participating species.

Mixture Density

Select a way to define the density from the **Mixture density** list — **Ideal gas** or **User defined**:

- For **Ideal gas**, the density is computed from the ideal gas law in the manner of:

$$\rho = \frac{pM}{R_g T}$$

  Here M is the mean molar mass of the mixture and R_g is the universal gas constant. The absolute pressure, p, and temperature, T, used corresponds to the ones defined in the **Model Inputs** section.
- For **User defined** enter a value or expression for the **Mixture density** ρ.

CONVECTION

Select the source of the **Velocity field u**:

- Select **User defined** to enter values or expressions for the velocity components. This input is always available.
- Select a velocity field defined by a Fluid Flow interface that solves for the velocity of the fluid. For example, select **Velocity field (spf)** to use the velocity field defined by in a Single-Phase Flow, Laminar Flow interface with `spf` as the Name.

When the interface is used in a reacting flow multiphysics coupling, the velocity is automatically defined and the input is disabled.

DIFFUSION

Specify the species molecular and thermal diffusivities in fluid phase in the manner described for the Fluid node.

To account for the effect of porosity in the diffusivities, select an **Effective diffusivity model** — **Millington and Quirk model**, **Bruggeman model**, **Tortuosity model**, or **No correction**. Using one of the first four models, the effective transport factor, f_e, is defined from the porosity and the fluid tortuosity factor in the manner of:

$$f_e = \frac{\varepsilon_p}{\tau_F} \tag{8-7}$$

For **No correction**, the effective transport factor is set to one.

- For the **Millington and Quirk model**, the effective transport factor is $\tau_F = \varepsilon_p^{-1/3}$.
- For the **Bruggeman model**, the effective transport factor is $\tau_F = \varepsilon_p^{-1/2}$.
- For the **Tortuosity model**, specify the tortuosity factor τ_F. Select either **Isotropic** to define a scalar value, or **Diagonal** or **Symmetric** to define anisotropic tensor values.

The species diffusivities and mobilities are automatically adjusted for porous media transport using the effective transport factor.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** checkbox is selected in the Transport Mechanisms section of the interface. Select the source of the **Electric potential** V:

- Select **User defined** to enter a value or expression for the electric potential.
- When present, select an electric potential defined by an AC/DC interface that is present in the model. For example, select **Electric potential (ec)** to use the electric field defined an Electric Currents interface `ec`.

Settings for the mobilities are needed for the **Mixture-averaged** and **Fick's law** diffusion models. By default the mobility is set to be calculated based on the species diffusivities (adjusted by the **Effective diffusivity model** in the **Diffusion** section) using the **Nernst-Einstein relation**. To manually specify the mobilities, select **User defined** for the mobility $u_{\mathrm{m,w}}$ and enter one value for each species.

The temperature (if you are using mobilities based or the Nernst–Einstein relation) is taken from the **Model Inputs** section.

Porous Matrix

This node defines the porosity, when modeling transport in a Porous Medium. The porosity corresponds to the volume fraction occupied by the species containing fluid.

- By default the porosity of the solid matrix, ε_{p}, is taken **From material**. The **Porous Matrix** node supports the use of a **Porous Material** added to the Materials branch. In this case the porosity is defined in the manner of

$$\varepsilon_{\mathrm{p}} = 1 - \sum_i \theta_{\mathrm{s},i} - \sum_i \theta_{\mathrm{imf},i}$$

  where $\theta_{\mathrm{s},i}$ and $\theta_{\mathrm{imf},i}$ are the volume fractions given in **Solid** and **Immobile Fluids** subnodes under the **Porous Material** node.
- Select **From pellet bed densities** to compute the porosity using the (dry bulk) **Bed density** ρ_{b} and the (single phase) **Pellet density** ρ_{pe}. The porosity is then defined from

$$\varepsilon_{\mathrm{p}} = 1 - \frac{\rho_{\mathrm{b}}}{\rho_{\mathrm{pe}}}$$

- For **User defined**, enter a value or expression for the porosity.

Electrode Surface Coupling

Use this node to define a flux boundary condition based on current densities of one or multiple Electrode Reaction (described in the Electrochemistry Module User's Guide) nodes in an Electrochemistry interface.

The flux is proportional to the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficients subnodes. The molar fluxes are multiplied by the species molar masses to obtain the corresponding mass fluxes.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity.

Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the mass flux from the electrode reactions. One example that may benefit from this is when modeling gas diffusion electrodes.

Reaction

Use the **Reaction** node to specify the reaction kinetics for a single homogeneous chemical reaction. The resulting mass source terms for the species involved in the reaction are automatically defined and added on the selected domains. For turbulent flow, the **Reaction** node includes the Eddy-dissipation turbulent-reactions model.

When licensed to use the Chemistry interface, multiple reactions can be defined at the same time, and the Reaction Sources node can be used to add the resulting mass sources.

See https://www.comsol.com/products/specifications/ for more details on availability.

REACTION RATE

Select a **Reaction rate** — **Automatic** (the default), or **User defined**. Selecting **Automatic** the laminar flow reaction rate is computed using the mass action law.

For **User defined**, input a custom expression or constants for the **Reaction rate** r.

Specify the reaction stoichiometry by entering values for the stoichiometric coefficients (dimensionless) of each species. Enter negative values for reactants and positive values for products.

RATE CONSTANTS

When the **Use Arrhenius expressions** checkbox is not selected, input custom expressions or constants for the **Forward rate constant** k^{f} and **Reverse rate constant** k^{r}.

When the **Use Arrhenius expressions** checkbox is selected, enter values for the following parameters of the forward and reverse reactions:

- **Forward frequency factor** A^{f} and **Reverse frequency factor** A^{r} (dimensionless)
- **Forward activation energy** E^{f} and **Reverse activation energy** E^{r}
- **Forward temperature exponent** n^{f} and **Reverse temperature exponent** n^{r} (dimensionless)

TURBULENT FLOW

Note this section is only available when licensed to the CFD Module (see https://www.comsol.com/products/specifications/).

When the **Turbulent-reaction model** is set to **None**, laminar flow is assumed and the reaction source terms are defined from the reaction stoichiometry and reaction rates prescribed.

When the **Turbulent-reaction model** is set to **Eddy-dissipation**, turbulent flow will be accounted for in the reaction mass sources in the manner described in The Reaction Source Term for Turbulent Flow. In this case, enter values for the **Turbulent reaction model parameters** α_{ED} and β_{ED} (dimensionless).

The **Eddy-dissipation** model also requires an estimation of the turbulent mixing time of the fluid flow turbulence. When a Fluid Flow interface defining it is present in the model, it can be selected from the **Turbulence time scale** list. For example, select **Turbulence time scale (spf/fp1)** to use the time scale defined by the **Fluid Properties** node `fp1` in a Turbulent Flow, k-ε interface with the **Name** set to `spf`.

REGULARIZATION

Select **Rate expression** in order to regularize the individual rate expressions that are added to each species. If the mass fraction for a reactant species ω_i becomes smaller than its **damping limit**, ω_i^{dl}, the rate expression added to species ω_i is reduced linearly. If $\omega_i \leq 0$ for a reactant species, the reaction rate contribution to that species is completely removed. Similarly, if the mass fraction for a product species ω_j becomes larger than $1 - \omega_j^{\mathrm{dl}}$, the rate expression added to that species is damped linearly. If $\omega_j \geq 1$ for a product species, the reaction rate contribution to that species is completely removed.

The default value for the **damping limit**, ω_i^{dl}, is 10^{-6}, which is appropriate for most applications, but can require adjustment when working with for example catalytic trace species.

Regularization of the rate expressions adds considerable stability to the reaction expressions, but should optimally only be used as a mean to reach convergence. If the regularization is active in too large parts of the domain, the mass balance can become affected since the regularization acts on the contributions to each individual species, not the reaction as a whole.

Reaction Sources

Use the **Reaction Sources** node to define mass source terms from one or more chemical reactions. Both homogeneous reactions as well as heterogeneous reactions occurring in a porous media can be studied. The node also includes the possibility to pick up automatically defined source term definitions from a Chemistry interface.

REACTIONS

Add an expression for the reaction mass source, R_i, for each individual species present, except for the one computed from the mass constraint (see Species). Enter a value or expression in the field for the corresponding species.

Select the **Mass transport to other phases** checkbox if mass is leaving or entering the fluid as a result of the reactions, for instance due to condensation or vaporization in a porous matrix. In this case the mass source for the species calculated from the mass constraint can also be specified. The net mass transfer corresponds to the sum of the mass sources for all species.

REACTING VOLUME

When specifying reaction sources for a species in porous media, the specified mass source may have the basis of the total volume, or the pore volume. For nonporous domains, the **Reacting Volume** setting has no impact.

- For **Total volume**, the reaction mass source expressions are specified per unit volume of the model domain.
- For **Pore volume**, the reaction mass source expressions are specified per unit volume pore space. In this case the reaction mass sources will be multiplied by the domain porosity ε_p (ε_p equals unity for nonporous domains).

Initial Values

The **Initial Values** node adds initial values for the mass fractions that can serve as an initial condition for a transient simulation, or as an initial guess for a nonlinear solver. If required, add additional **Initial Values** nodes from the **Physics** toolbar.

INITIAL VALUES

The initial mass fractions can be specified using a number of quantities. Select the type of input from the **Mixture specification** list. Select:

- **Mass fractions** (the default) to enter mass fractions ($\omega_{0,\omega 1}$ for example)
- **Mole fractions** to enter mole fractions ($x_{0,\omega 1}$ for example)
- **Molar concentrations** (SI unit: $\mathrm{mol/m^3}$) to enter molar concentrations ($c_{0,\omega 1}$ for example)
- **Number densities** (SI unit: $1/\mathrm{m^3}$) to enter number densities ($n_{0,\omega 1}$ for example)
- **Densities** (SI unit: $\mathrm{kg/m^3}$) to enter densities ($\rho_{0,\omega 1}$ for example)

Enter a value or expression in the field for each species except for the one computed from the mass constraint.

INITIAL MIXTURE DENSITY

When the selecting **Molar concentrations**, **Number densities**, or **Densities** are selected from the **Mixture specification** list, the should also be specified. Select **Ideal gas** or **User defined** from the **Initial mixture density** list.

- For **Ideal gas**, also specify the **Initial pressure** p_0 and the **Initial Temperature** T_0. Note that dependent variables solved for are evaluated to zero for initial values. When

solving for pressure or temperature together with the mass fractions, apply the initial values from the corresponding interfaces here as well.

- For **User defined**, input a custom for the **Initial mixture density** ρ_{m0}.

Mass Fraction

The **Mass Fraction** node adds boundary conditions for the species mass fractions. For example, the following condition specifies the mass fraction of species *i:* $\omega_i = \omega_{i,0}$.

Set the mass fractions of all species except the one computed from the mass constraint. This ensures that the sum of the mass fractions is equal to one (see Species). This node is available for exterior and interior boundaries.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

MASS FRACTION

Specify the mass fraction for each species individually. Select the checkbox for the species to specify the mass fraction, and enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the checkbox for the mass fraction of that species.

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity.

Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the prescribed mass fractions. Examples of cases that may benefit from this are, for example, when modeling surface reactions or phase change on an exterior boundary.

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

Flux

The **Flux** node is available on exterior boundaries and can be used to specify the mass flux. The boundary mass flux for each species is defined in the manner of

$$-\mathbf{n} \cdot \mathbf{j}_i = j_{0,i} \tag{8-8}$$

where $\mathbf{n}$ denotes the outward pointing normal of the boundary. The prescribed flux $j_{0,i}$ can contain an arbitrary flux expression. It can, for example, be used to represent a *heterogeneous reaction* or a separation process occurring at the boundary. The flux can, for example, be a function of ω_i, the temperature, the pressure or even the electric potential.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

CONVECTION

By default, the flux due to diffusion and migration in an electric field is prescribed. This is the appropriate flux condition when the relative velocity at the boundary is zero. When the fluid velocity is not equal to that of the boundary, for example due to a fluid injection, it is often convenient to prescribe the total flux including convection. To do so select **Include** in the **Convection** section. In this case the prescribed flux is defined as:

$$-\mathbf{n} \cdot (\mathbf{j}_i + \rho \mathbf{u} \omega_i) = j_0$$

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity.

Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the prescribed flux. Examples of cases that benefit from this are for example when modeling surface reactions or phase change on an exterior boundary. The Stefan velocity represents the mixture velocity resulting from mass fluxes at the wall. This section is not available when **Include** is selected in the **Convection** section.

INWARD FLUX

Specify the **Inward flux** for each species individually. Select the checkbox for the species to prescribe a flux for and enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the checkbox for the flux of that species. Use a positive value for an inward flux.

External convection

Set **Flux type** to **External convection** to prescribe a mass flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$j_{0,i} = k_{\omega,i}(\omega_{b,i} - \omega_i) \tag{8-9}$$

where $k_{\omega,i}$ is a mass transfer coefficient and $\omega_{b,i}$ is the bulk mass fraction, the typical mass fraction far into the surrounding exterior domain.

Inflow

The **Inflow** node adds a boundary condition for an inflow boundary, defining the composition of the mixture. The node is available for exterior boundaries. The mixture composition can be specified using the following quantities:

- Mass fractions: $\omega_i = \omega_{0,i}$
- The mole fraction: $x_i = x_{0,i}$
- The molar concentration: $c_i = c_{0,i}$
- The number density, which describes the number of particles per volume: $n_i = n_{0,i}$
- The density: $\rho_i = \rho_{0,i}$
- The mass flow rates.

The node requires input for all species. (The Mass Fraction node can be used to specify boundary mass fractions for a subset of the active species in the interface.)

INFLOW

Select a **Mixture specification**:

- **Mass fractions** (the default) to enter mass fractions ($\omega_{0,\omega1}$, for example)
- **Mole fractions** to enter mole fractions ($x_{0,\omega1}$ for example)
- **Molar concentrations** (SI unit: $\mathrm{mol/m^3}$) to enter molar concentrations ($c_{0,\omega1}$, for example)
- **Number densities** (SI unit: $1/\mathrm{m^3}$) to enter number densities ($n_{0,\omega1}$, for example)
- **Densities** (SI unit: $\mathrm{kg/m^3}$) to enter densities ($\rho_{0,\omega1}$, for example)
- **Mass flow rates** (SI unit: kg/s) to enter the total mass flow over the boundary ($J_{in,\omega1}$, for example)

Enter a value or expression in the field for each species except for the one computed from the mass constraint.

CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

No Flux

The **No Flux** node is the default boundary condition available for exterior boundaries. It should be used on boundaries across which there is no mass flux, typically exterior solid walls where no surface reactions occur. The condition applied for each species corresponds to

$$-\mathbf{n} \cdot \mathbf{j}_i = 0$$

where $\mathbf{n}$ denotes the outward pointing normal of the boundary.

Out-of-Plane Flux

The out-of-plane flux node is used to prescribe a flux in an out-of-plane domain, and it can be used to reduce a model geometry to 2D, or even 1D, when the variation of mass fraction is small in one or more directions. This could be the case for example when the object to model is thin or slender. Figure 8-1shows examples of possible situations in which this type of geometry reduction can be applied.

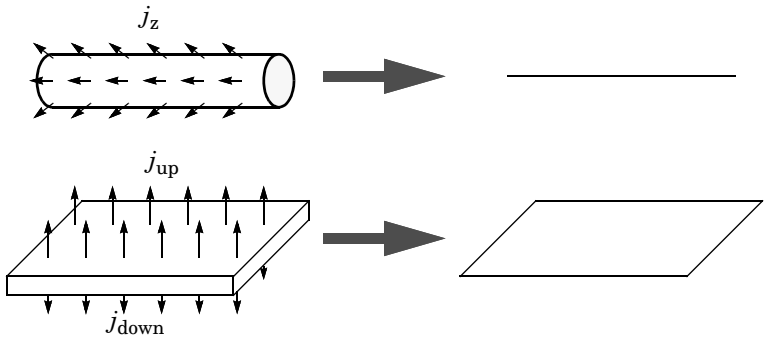

Figure 8-2: Geometry reduction from 3D to 1D (top) and from 3D to 2D (bottom).

For a 1D component this node adds a single out-of-plane mass flux $j_{0,z,i}$ for species i. For a 2D component two fluxes can be prescribed for each species; $j_{0,u,i}$ for the upside of the domain, and $j_{0,d,i}$ for the downside of the domain.

The fluxes are added as a source contribution to the right-hand side of the transport equation. For example, in 2D components with diffusion, convection, and out-of-plane flux present, the mass transfer of species i is defined by the mass conservation equation

$$\rho\frac{\partial}{\partial t}(\omega_i) + \rho(\mathbf{u}\cdot\nabla)\omega_i + \nabla\cdot\mathbf{j}_i = R_i + S_{\mathrm{opf},i}, \tag{8-10}$$

where $S_{\mathrm{opf},i}$ is the out-of-plane source for species i

$$S_{\mathrm{opf},i} = \frac{j_{0,i}}{d_z} = \frac{j_{0,\mathrm{u},i} + j_{0,\mathrm{d},i}}{d_z} \quad .$$

For external mass transfer on the upside and the downside of the domain, the out-of-plane flux is

$$j_{0,i} = k_{w,\mathrm{u},i}(w_{\mathrm{b},\mathrm{u},i} - w_i) + k_{w,\mathrm{d},i}(w_{\mathrm{b},\mathrm{d},i} - w_i)$$

where $k_{\omega,i}$ is a mass transfer coefficient and $\omega_{\mathrm{b},i}$ is the bulk mass fraction, the typical mass fraction far into the surrounding exterior domain. The prescribed flux, j_0, can include any arbitrary user-specified expressions. It can be a constant or a function of a dependent variable or independent variables.

UPSIDE INWARD FLUX

For 1D components, enter the **cross-sectional perimeter** P_c to get the out-of-plane flux

$$j_{0,i} = P_c j_{0,z,i} \quad .$$

The default value of P_c is the circumference. Either keep the default value, for a circular cross-section shape, or edit the value to get a user-defined shape of the out-of-plane cross-section.

The available options are **General inward flux** and **External convection**. Specify the **Inward flux** for each species individually. Select the **Species** checkbox for the species for which to specify the flux, and enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the checkbox for the flux of that species. Use a positive value for an inward flux.

Set **Flux type** to **External convection** to prescribe a mass flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$j_{0,i} = k_{\omega,i}(\omega_{\mathrm{b},i} - \omega_i)$$

where $k_{\omega,i}$ is a mass transfer coefficient and $\omega_{\mathrm{b},i}$ is the bulk mass fraction, the typical mass fraction far into the surrounding exterior domain.

DOWNSIDE INWARD FLUX

The available options are **General inward flux** and **External convection**. The settings are the same as for the Upside Inward Flux section.

FURTHER READING

For an example of using the Out-of-Plane Flux node, see this application example:

Cross-Flow Mass Transfer in a Thin Domain: Application Library path **Chemical_Reaction_Engineering_Module/Tutorials/thin_domain**

Outflow

The **Outflow** node is the preferred boundary condition at outlets where the species are to be transported out of the model domain. It is useful, for example, in mass transport models where it is assumed that convection is the dominating effect driving the mass flow through the outflow boundary. This node is available for exterior boundaries. The boundary condition is applied to all species and corresponds to one of the following equations depending on the selected diffusion model:

- For the Mixture-Averaged Diffusion Model:

$$-\mathbf{n} \cdot \rho D_i^m \nabla \omega_i = 0$$

- For the Fick's Law Diffusion Model:

$$-\mathbf{n} \cdot \rho D_i^f \nabla \omega_i = 0$$

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric; that is, there is no mass flux in the normal direction across the boundary:

$$-\mathbf{n} \cdot \mathbf{N} = -\mathbf{n} \cdot (\rho \omega_i \mathbf{u} + \mathbf{j}_i) = 0$$

This boundary condition is identical to the No Flux node, but applies to all species and cannot be applied to individual species. The Symmetry node is available for exterior boundaries.

Flux Discontinuity

The **Flux Discontinuity** node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n}\cdot(\mathbf{N}_\mathrm{d}-\mathbf{N}_\mathrm{u}) = N_0 \qquad \mathbf{N} = (\rho\omega_i\mathbf{u}+\mathbf{j}_i)$$

where the value of N_0 specifies the size of the flux jump evaluated from the down to the upside of the boundary.

FLUX DISCONTINUITY

Specify the jump in species mass flux. Use a positive value for increasing flux when going from the downside to the upside of the boundary. The boundary normal points in the direction from the downside to the upside of an interior boundary and can be plotted for visualization.

Select the **Species** checkboxes to specify a flux discontinuity, and enter a value or expression for the **Flux discontinuity** N_0 (SI unit: kg/(m^2·s)) in the corresponding field, $N_{0,\,\mathrm{w1}}$, for example. To use a different boundary condition for a specific species, click to clear the checkbox for the flux discontinuity of that species.

Open Boundary

Use the **Open Boundary** node to set up mass transport across boundaries where both convective inflow and outflow can occur. Use the node to specify an exterior species composition on parts of the boundary where fluid flows into the domain. A condition equivalent to the Outflow node applies to the parts of the boundary where fluid flows out of the domain. The direction of the flow across the boundary is typically calculated by a Fluid Flow interface and is entered as Model Inputs.

EXTERIOR COMPOSITION

Enter a value or expression for the species composition. Select:

- **Mass fractions** (the default) to enter mass fractions ($\omega_{0,\omega1}$, for example)
- **Mole fractions** to enter mole fractions ($x_{0,\omega1}$, for example)
- **Molar concentrations** (SI unit: mol/m^3) to enter molar concentrations ($c_{0,\omega1}$, for example)

- **Number densities** (SI unit: $1/\mathrm{m}^3$) to enter number densities ($n_{0,\omega 1}$, for example) and to describe the number of particles per volume $n = n_0$
- **Densities** (SI unit: kg/m^3) to enter densities ($\rho_{0,\omega 1}$, for example)

	A concentration quantity other than the mass fractions can only be used when all species are defined.

Equilibrium Reaction

Use this node to model a reaction where the kinetics is assumed so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the reaction rate R_{eq}) to fulfill the equilibrium condition at all times in all space coordinates.

	This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EQUILIBRIUM CONDITION

Selecting **Equilibrium constant** in the list, the following equilibrium condition based on the species activities and the law of mass action is used

$$K_{\mathrm{eq}} = \frac{\prod_{i \in \text{ products}} a_i^{\nu_i}}{\prod_{i \in \text{ reactants}} a_i^{-\nu_i}}$$

where ν_i are the stoichiometric coefficients and the species activities are defined from the concentration, c_i, and the unit activity concentration c_{a0}.

$$a_i = \frac{c_i}{c_{\mathrm{a0}}}$$

Enter a value or expression for the dimensionless **Equilibrium constant** K_{eq}, and the **Unit activity concentration** C_{a0}.

Select **User defined** from the list to instead enter a manually defined **Equilibrium expression** E_{eq}.

STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient ν for all participating species. Use negative values for reactants and positive values for products in the modeled reaction. Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium Reaction** node.

Surface Equilibrium Reaction

Use this node to model an equilibrium reaction on a boundary (surface). The kinetics of the reaction is assumed so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the mass flux J_{eq}) to fulfill the equilibrium condition at all times in all space coordinates along the boundary.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The settings for this node are the same as for Equilibrium Reaction except for the setting in the section below.

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity. Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the prescribed mass fractions. Examples of cases that may benefit from this are for example when modeling surface reactions or phase change on an exterior boundary.

The Vapor Flow Multiphysics Interfaces

The Vapor Flow multiphysics interfaces are predefined multiphysics interfaces that couple fluid flow with mass transport in vapor mixtures. The interfaces require a license for the Chemical Reaction Engineering Module. When also licensed to the CFD Module the functionality is extended with interfaces for modeling turbulent flow.

Selecting a Vapor Flow multiphysics interface under the **Chemical Species Transport** > **Vapor Flow** branch of the **Model Wizard**, a Fluid Flow interface and a **Transport of Concentrated Species in Vapor** interface are added to the Model Builder. In addition, the **Multiphysics** node is added, which includes the multiphysics coupling feature **Reacting Flow**. The **Reacting Flow** feature predefines and controls the couplings between the separate interfaces in order to facilitate easy set up of models. See The Vapor–Liquid Equilibrium Multiphysics Interfaces in the *Chemical Reaction Engineering Module User's Guide* for more information on the included interfaces.

The Transport of Concentrated Species in Vapor Interface (in the *Chemical Reaction Engineering Module User's Guide*) includes three dedicated boundary features for vapor transfer. The **Vapor Inflow** feature can be used to prescribe inflow conditions resulting from an upstream system involving a liquid. The **Vapor–Liquid Interface** feature ca n be used to model condensation and evaporation to or from a gas mixture in contact with a liquid. In the case of a liquid with multiple components, the **Vapor–Liquid-Mixture Interface** can be used to also model the composition in the liquid.

The Reacting Flow, Concentrated Species Multiphysics Interfaces

The CFD Module includes predefined multiphysics interfaces that couple fluid flow with mass transport and reactions.

Selecting a multiphysics interface under the **Chemical Species Transport** > **Reacting Flow** branch of the **Model Wizard** or **Add Physics** windows, one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) and a **Transport of Concentrated Species** interface are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature **Reacting Flow**. The **Reacting Flow** feature predefines and controls the couplings between the separate interfaces in order to facilitate easy set up of models.

In this section:

- The Reacting Laminar Flow, Concentrated Species Interface
- The Reacting Turbulent Flow, k-ε, Concentrated Species Interface
- The Reacting Turbulent Flow, k-ω, Concentrated Species Interface
- The Reacting Turbulent Flow, SST, Concentrated Species Interface
- The Reacting Turbulent Flow, Low Re k-ε, Concentrated Species Interface
- The Reacting Flow Coupling Feature
- Physics Interface Features

The Reacting Laminar Flow, Concentrated Species Interface

The **Reacting Laminar Flow** ( ) multiphysics interface is used to simulate laminar flow coupled to species transport in a gas or liquid.

It combines the **Laminar Flow**, and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport. The fluid flow can either be free flow or flow in a porous medium. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

ON THE CONSTITUENT PHYSICS INTERFACES

The equations solved by the **Laminar Flow** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. A **Fluid Properties** feature is active by default on the entire interface selection. A **Porous Medium** feature can be added in order to model flow in porous media by solving the Brinkman equations.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The **Reacting Laminar Flow** interface triggers pseudo time stepping for the flow equations when **Use pseudo time stepping for stationary equation form** in the **Fluid Flow** interface is set to **Automatic from physics**.

The Reacting Turbulent Flow, k-ε, Concentrated Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow, k-ε** and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples the fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

ON THE CONSTITUENT PHYSICS INTERFACES

The equations solved by the **Turbulent Flow, k-ε** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled

using wall functions, and reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, k-ω, Concentrated Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow k-ω** and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

ON THE CONSTITUENT PHYSICS INTERFACES

The equations solved by the **Turbulent Flow k-ω** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the Wilcox revised k-ω model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions, and reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, SST, Concentrated Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow, SST** and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

ON THE CONSTITUENT PHYSICS INTERFACES

The equations solved by the **Turbulent Flow, SST** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the SST model. The SST model is a low-Reynolds number model which means that it resolves the velocity, pressure, and mass fractions all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The SST model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, Low Re k-ε, Concentrated Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow, Low Re k-ε** and **Transport of Concentrated Species** interfaces. **The Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

ON THE CONSTITUENT PHYSICS INTERFACES

The equations solved by the **Turbulent Flow, Low Re k-ε** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the AKN low-Reynolds number k-ε model. The low-Reynolds number model resolves the velocity, pressure, and mass fractions all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The

AKN model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Flow Coupling Feature

Use the **Reacting Flow** ( ) multiphysics coupling to simulate mass transport and reactions in a gas or liquid mixture where the fluid flow can be dependent on the mixture composition. When a **Heat Transfer** and a **Chemistry** interface are selected, use this coupling to simulate heat transfer additionally to mass transport and reactions.

The coupling adds the heat source of reaction when a heat transfer interface is selected. No additional heat source needs to be defined to account for it in the heat transfer interface. It also accounts for the multiphysics stabilization terms, for work due to pressure forces and viscous dissipation.

Select a **Fluid Flow** interface and a **Species transport** interface to couple fluid flow with mass transport. **Chemistry** and **Heat Transfer** are optional. They can be set to **None** when the coupling is used to simulate isothermal mixtures.

When a **Chemistry** interface is selected and **Heat Transfer** is set to **None**, fluid properties are taken from the Chemistry interface. Set the **Temperature** to evaluate the fluid properties synchronized with all the physics interfaces at the given temperature.

Select a **Chemistry** interface and **Heat Transfer** interface in order to account for the heat of reaction, enthalpy diffusion, viscous heating and mass fluxes contributing to the heat and energy balance.

When **Chemistry** is set to **None** and a **Heat Transfer** interface is selected, the coupling is solved in the same way as when no Heat Transfer interface is selected. Thermodynamic properties are required by the Heat Transfer interface.

The pressure, velocity, and temperature variables of the **Reacting Flow** coupling node are set to the **Common Model Input** values of the **Default Model Inputs** node on the complementary selection, that is, all domains except those from the **Selection** list. It allows to couple multiple fluid flow or transport of species interfaces with a single heat transfer interface. See Default Model Inputs in the *COMSOL Multiphysics Reference Manual* for details.

DOMAIN LEVEL SYNCHRONIZATION

The **Reacting Flow** coupling synchronizes the features from a Chemistry interface, Heat Transfer interface, Single-Phase Flow, or Brinkman Equations, interface and a Transport of Concentrated Species interface. When the Chemistry interface is not selected, the density in the Single-Phase Flow interface is automatically synchronized to the one defined by the Transport of Concentrated Species interface.

The velocity field used by the Transport of Concentrated Species interface and Heat Transfer interface is synchronized to the one computed in the Single-Phase Flow interface.

When a Chemistry interface is selected, the **Reacting Flow** coupling synchronizes the definition of the thermal conductivity, density, heat capacity, enthalpy, and dynamic viscosity with the other coupled physics interfaces. The reference temperature is taken from the Heat Transfer interface.

THE STEFAN VELOCITY

The **Reacting Flow** coupling feature automatically couples mass transfer on boundaries and applies a corresponding velocity contribution for the flow. Prescribing a net mass boundary flux in the **Transport of Concentrated Species** interface, either using a **Flux** or **Mass Fraction** feature, the **Reacting Flow** feature computes The Stefan Velocity and applies this in **Wall** features using the same selection.

MASS TRANSFER TO OTHER PHASES IN POROUS MEDIA

When coupled to the **Brinkman Equations** interface, the **Reacting Flow** node automatically computes the net mass source or sink in a **Reactions** (when **Mass transfer to other phases is enabled**) node in the **Transport of Concentrated Species** interface and adds the corresponding source/sink to the momentum equations of the **Fluid and Matrix Properties** domains.

TURBULENT MASS TRANSFER

When a turbulence model is used, the **Reacting Flow** coupling applies turbulence modeling for the mass transport in the following manners:

- Turbulent heat transfer and mass transport are added, defined from the turbulent viscosity and a turbulent Schmidt number (for more information, see Turbulent Mass Transport Models).
- Temperature and mass transport wall functions. When a turbulence model using wall functions is used for the fluid flow, the Reacting Flow coupling automatically adds wall functions for the temperature and mass transport on the same boundaries (for more information, see Mass Transport Wall Functions).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `nirf1`.

DOMAIN SELECTION

The **Reacting Flow** coupling is automatically defined on the intersection of the selections for the coupled interfaces. When modeling porous media transport a **Porous Medium** feature, applied on the same domains, is needed in all coupled transport interfaces. **Reacting Flow** coupling supports porous media transport in **Fluid flow** and **Species transport** interfaces.

The **Selection** list displays the domains where the coupling feature is active.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow, Species transport, Chemistry, Heat Transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from a list to uncouple the node from a physics interface.

Click the **Go to Source** buttons ( ) to move to the main physics interface node for the selected physics interface.

Click the **Show or Hide Physics Properties Settings** button ( ) to toggle the display of physics properties settings affecting the coupling feature. When a turbulence model is used, turbulent heat and mass transfer is automatically accounted for (see the settings in the **Turbulence** section below). Using Reacting Flow, the heat and mass transfer treatment at walls follows that applied for the fluid flow. Therefore the **Wall treatment** setting is also displayed when using a turbulence model. For more information on turbulent mass transfer at walls, see the section Mass Transport Wall Functions in the *CFD Module User's Guide*.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow**, **Species transport**, **Chemistry** and **Heat Transfer** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

MASS TRANSPORT TURBULENCE MODEL

When the fluid flow interface uses a turbulence model, select an option from the **Mass transport turbulence model** list — **Kays-Crawford**, **High Schmidt Number**, or **User-defined turbulent Schmidt number**.

For **User-defined turbulent Schmidt number**, enter a **Turbulent Schmidt number** Sc_T (dimensionless).

The turbulent mass transfer added to the mass fraction equations is defined as

$$N_{i,\mathrm{T}} = -\frac{\mu_\mathrm{T}}{\mathrm{Sc}_\mathrm{T}}\nabla\omega_i$$

where μ_T is the turbulent viscosity defined by the flow interface, and the turbulent Schmidt number, Sc_T, depends on the **Mass transport turbulence model** used.

HEAT TRANSFER TURBULENCE MODEL

This section is available when a Heat Transfer interface is selected and the fluid flow interface uses a turbulence model. Select an option from the **Heat transport turbulence model** list: **Kays-Crawford** (the default), **Extended Kays-Crawford**, or **User-defined turbulent Prandtl number**.

For **Extended Kays-Crawford**, enter a **Reynolds number at infinity** Re_inf (dimensionless).

For **User-defined turbulent Prandtl number**, enter a **Turbulent Prandtl number** Pr_T (dimensionless).

When the flow interface uses a RANS turbulence model, the conductive heat flux is defined as

$$q = -(k + k_\mathrm{T})\nabla T$$

with the turbulent thermal conductivity defined as

$$k_\mathrm{T} = \frac{\mu_\mathrm{T} C_p}{\mathrm{Pr}_\mathrm{T}}$$

where μ_T is defined by the flow interface, and Pr_T depends on the **Heat transport turbulence model**. See Turbulent Conductivity for details.

The **Turbulence model type** used by the fluid flow interface can be displayed by selecting the **Show or Hide Physics Property Settings** button at the right of the **Fluid flow** list.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

LAMINAR FLOW

The available physics features for The Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow in the *COMSOL Multiphysics Reference Manual*.

TURBULENT FLOW, k-ε

The available physics features for The Turbulent Flow, k-ε interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ω

The available physics features for The Turbulent Flow, k-ω interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE k-ε

The available physics features for The Turbulent Flow, Low Re k-ε interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for The Transport of Concentrated Species interface are listed in the section Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface.

The Reacting Flow, Diluted Species Multiphysics Interfaces

Reacting Flow, Diluted Species is a predefined multiphysics interface, available in the CFD Module, that couples fluid flow with mass transport and reactions.

Selecting **Laminar Flow, Diluted Species** under the **Chemical Species Transport** > **Reacting Flow** branch of the **Model Wizard** or **Add Physics** windows, a **Laminar Flow** interface and a **Transport of Diluted Species** interface are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature **Reacting Flow, Diluted Species**. The **Reacting Flow, Diluted Species** feature predefines and controls the couplings between the separate interfaces in order to facilitate easy set up of models.

In this section:

- The Reacting Laminar Flow, Diluted Species Interface
- The Reacting Turbulent Flow, k-ε, Diluted Species Interface
- The Reacting Turbulent Flow, k-ω, Diluted Species Interface
- The Reacting Turbulent Flow, SST, Diluted Species Interface
- The Reacting Turbulent Flow, Low Re k-ε, Diluted Species Interface
- The Reacting Flow, Diluted Species Coupling Feature
- Physics Interface Features

The Reacting Laminar Flow, Diluted Species Interface

The **Reacting Laminar Flow, Diluted Species** multiphysics interface ( ) is used to simulate laminar flow coupled to transport of dilute solutes in a gas or liquid.

It combines the **Laminar Flow**, and **Transport of Diluted Species** interfaces. The **Reacting Flow, Diluted Species** multiphysics coupling, which is added automatically, couples fluid flow and mass transport. The fluid flow can either be free flow or flow in a porous medium. The mass transfer solves for the development of one or several solutes dissolved in a gas or liquid solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Laminar Flow** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. A **Fluid Properties** feature is active by default on the entire interface selection. A **Porous Medium** feature can be added in order to model flow in porous media by solving the Brinkman equations.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The Reacting Turbulent Flow, k-ε, Diluted Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to transport of dilute solutes present in a gas or liquid.

It combines the **Turbulent Flow, k-ε** and **Transport of Diluted Species** interfaces. The **Reacting Flow, Diluted Species** multiphysics coupling, which is added automatically, couples the fluid flow and mass transport and applies turbulence modeling for the mass transport. The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, k-ε** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions.

The Reacting Turbulent Flow, k-ω, Diluted Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to transport of dilute solutes present in a gas or liquid.

It combines the **Turbulent Flow k-ω** and **Transport of Diluted Species** interfaces. The **Reacting Flow, Diluted Species** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow k-ω** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the Wilcox revised k-ω model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions.

The Reacting Turbulent Flow, SST, Diluted Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to transport of dilute solutes present in a gas or liquid.

It combines the **Turbulent Flow, SST** and **Transport of Diluted Species** interfaces. The **Reacting Flow, Diluted Species** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, SST** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the SST model. The SST model is a low-Reynolds number model which means that it resolves the velocity, pressure, and concentrations all the way down to the wall. For that reason this physics

interface is suited for studying mass transfer at high Schmidt numbers. The SST model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions.

The Reacting Turbulent Flow, Low Re k-ε, Diluted Species Interface

This multiphysics interface ( ) is used to simulate flow in the turbulent regime coupled to transport of dilute solutes present in a gas or liquid.

It combines the **Turbulent Flow, Low Re k-ε** and **Transport of Diluted Species** interfaces. The **Reacting Flow, Diluted Species** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, Low Re k-ε** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the AKN low-Reynolds number k-ε model. The low-Reynolds number model resolves the velocity, pressure, and concentrations all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The AKN model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions.

The Reacting Flow, Diluted Species Coupling Feature

The **Reacting Flow, Diluted Species** ( ) multiphysics coupling is used to simulate mass transport and reactions in a gas or liquid.

DOMAIN LEVEL SYNCHRONIZATION

The **Reacting Flow, Diluted Species** coupling synchronizes the features from a Single-Phase Flow, or Brinkman Equations, interface and a Transport of Diluted Species interface. When added, the velocity field used by the Transport of Diluted Species interface is synchronized to the one computed in the fluid flow interface.

TURBULENT MASS TRANSFER

When a turbulence model is used, the **Reacting Flow, Diluted Species** coupling applies turbulence modeling for the mass transport in the following manners:

- Turbulent mass transport is added, defined from the turbulent viscosity and a turbulent Schmidt number (for more information, see Turbulent Mass Transport Models).
- Mass transport wall functions. When a turbulence model using wall functions is used for the fluid flow, the Reacting Flow coupling automatically adds wall functions for the mass transport on the same boundaries (for more information, see Mass Transport Wall Functions).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `rfd1`.

DOMAIN SELECTION

The **Reacting Flow, Diluted Species** coupling is automatically defined on the intersection of the selections for the coupled interfaces.

The **Selection** list displays the domains where the coupling feature is active.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Species transport** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (macOS and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Laminar Flow** is deleted, then the **Fluid Flow** list defaults to **None** as there is nothing to couple to.

Click the **Go to Source** buttons ( ) to move to the main physics interface node for the selected physics interface.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Species transport** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

TURBULENCE

When the fluid flow interface uses a turbulence model, select an option from the **Mass transport turbulence model** list — **Kays–Crawford**, **High Schmidt Number**, or **User-defined turbulent Schmidt number**.

For **User-defined turbulent Schmidt number**, enter a **Turbulent Schmidt number** Sc_T (dimensionless).

The turbulent mass transfer added to the concentration equations is defined as

$$\mathbf{J}_{T,i} = -\frac{\mu_T}{Sc_T}\nabla c_i$$

where μ_T is the turbulent viscosity defined by the flow interface, and the turbulent Schmidt number, Sc_T, depends on the **Mass transport turbulence model** used.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (macOS or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

LAMINAR FLOW

The available physics features for The Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ε

The available physics features for The Turbulent Flow, k-ε interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-ω

The available physics features for The Turbulent Flow, k-ω interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE k-ε

The available physics features for The Turbulent Flow, Low Re k-ε interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TRANSPORT OF DILUTED SPECIES

The available physics features for The Transport of Diluted Species interface are listed in the section Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface in the *Chemical Reaction Engineering Module User's Guide*.

The Reacting Flow in Porous Media Interfaces

The CFD Module includes two predefined multiphysics interface that couples fluid flow in porous media with mass transport and reactions in porous media.

Selecting a multiphysics interface under the **Chemical Species Transport** > **Reacting Flow in Porous Media** branch of the **Model Wizard** or **Add Physics** windows, a **Brinkman Equations** interface combined with either the **Transport of Diluted Species in Porous Media** interface or the **Transport of Concentrated Species** interfaces are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature. The multiphysics coupling feature controls the coupling between the separate interfaces in order to facilitate easy setup of models.

In this section:

- The Reacting Flow in Porous Media, Transport of Diluted Species Interface
- The Reacting Flow in Porous Media, Transport of Concentrated Species Interface
- The Reacting Flow, Diluted Species Coupling Feature
- The Reacting Flow Coupling Feature
- Physics Interface Features

The Reacting Flow in Porous Media, Transport of Diluted Species Interface

The **Reacting Flow in Porous Media, Transport of Diluted Species** interface ( ) is used to study the flow and chemical composition of a gas or liquid moving through the interstices of a porous medium.

It combines the **Brinkman Equations**, and **Transport of Diluted Species in Porous Media** interfaces. The **Reacting Flow, Diluted Species** multiphysics coupling feature, which is added automatically, couples the fluid flow and mass transport. A **Porous Material** node, including a **Fluid** and a **Solid** subnode, is also added to the component.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi, and 3D.

On the constituent physics interfaces:

The **Brinkman Equations** interface computes the fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. A **Porous Medium** feature is active by default on the entire interface selection.

The **Transport of Diluted Species in Porous Media** interface computes the species concentration in free and porous media, assuming that the species are solutes, dissolved in a solvent of significantly higher concentration. A **Porous Medium** feature is active by default on the entire interface selection.

The Reacting Flow in Porous Media, Transport of Concentrated Species Interface

The **Reacting Flow in Porous Media, Transport of Concentrated Species** interface ( ) is used to study the flow and chemical composition of a gas or liquid moving through the interstices of a porous medium. The fluid can consist of a mixture of species where the individual concentrations are of comparable order of magnitude.

It combines the **Brinkman Equations**, and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling feature, which is added automatically, couples the fluid flow and mass transport. A **Porous Material** node is also added to the component.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi, and 3D.

On the constituent physics interfaces:

The **Brinkman Equations** interface computes the fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. A **Porous Medium** feature is active by default on the entire interface selection.

The **Transport of Concentrated Species in Porous Media** interface solves for an arbitrary number of mass fractions in free and porous media. In the current multiphysics interface a **Porous Medium** feature is active by default on the entire interface selection.

The Reacting Flow, Diluted Species Coupling Feature

For the settings of this feature see The Reacting Flow, Diluted Species Coupling Feature in the *Chemical Reaction Engineering Module User's Guide*.

The Reacting Flow Coupling Feature

For the settings of this feature see The Reacting Flow Coupling Feature in the *Chemical Reaction Engineering Module User's Guide*.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

BRINKMAN EQUATIONS

The available physics features for The Brinkman Equations interface are listed in the Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface section in the *CFD Module User's Guide*.

TRANSPORT OF DILUTED SPECIES

The available physics features for The Transport of Diluted Species interface are listed in the Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface section.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for The Transport of Concentrated Species interface are listed in the Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface section.

The Nonisothermal Reacting Flow Multiphysics Interfaces

Nonisothermal Reacting Flow is a predefined multiphysics interface, available in the CFD Module, that couples fluid flow and heat transfer with species transport and reactions.

Selecting an entry in the **Chemical Species Transport** > **Nonisothermal Reacting Flow** branch of the **Model Wizard**, or **Add Physics** windows, the following four physics interfaces are added to the Model Builder:

- **Chemistry**
- **Transport of Concentrated Species**
- **Laminar Flow**, or a turbulent flow equivalent like **Turbulent Flow, k-ε**.
- **Heat Transfer in Fluids**

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature **Reacting Flow**. The **Reacting Flow** feature predefines and controls the couplings between the separate interfaces in order to facilitate set up of models.

In this section:

- The Nonisothermal Reacting Laminar Flow Interface
- The Nonisothermal Reacting Turbulent Flow, k-ε Interface
- The Nonisothermal Reacting Turbulent Flow, k-ω Interface
- The Nonisothermal Reacting Turbulent Flow, SST Interface
- The Nonisothermal Reacting Turbulent Flow, Low Re k-ε Interface
- The Reacting Flow Coupling Feature
- Physics Interface Features

The Nonisothermal Reacting Laminar Flow Interface

The **Nonisothermal Reacting Laminar Flow** ( ) multiphysics interface is used to simulate laminar flow and heat transfer coupled to species transport in a gas or liquid moving either in a free flow or through the interstices of a porous medium. This interface requires a license for either the Chemical Reaction Engineering Module, the Battery Design Module, or the Fuel Cell & Electrolyzer Module.

It combines the **Chemistry**, **Transport of Concentrated Species**, **Laminar Flow**, and **Heat Transfer in Fluids** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow, heat transfer, and mass transfer. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The multiphysics coupling takes into account the heat of reaction in the fluid and at the surface of a porous catalyst, enthalpy diffusion, and contributing mass fluxes. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. A **Transport Properties** feature is active by default on the entire interface selection

The equations solved by the **Laminar Flow** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. A **Fluid Properties** feature is active by default on the entire interface selection.

The **Heat Transfer** interface solves for conservation of energy. A **Fluid** feature is active by default on the entire interface selection.

The Nonisothermal Reacting Turbulent Flow, k-ε Interface

The **Nonisothermal Reacting Turbulent Flow, k-ε** ( ) multiphysics interface is used to simulate flow in the turbulent regime, heat transfer, and species transport and in a gas or liquid moving either in a free flow or through the interstices of a porous medium. This interface requires a license for either the Chemical Reaction Engineering Module, the Battery Design Module, or the Fuel Cell & Electrolyzer Module.

It combines the **Chemistry**, **Transport of Concentrated Species**, **Turbulent Flow, k-ε**, and **Heat Transfer in Fluids** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow, heat transfer and mass transfer. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The multiphysics coupling takes into account the heat of reaction in the fluid and at the surface of a porous catalyst, enthalpy diffusion, and contributing mass fluxes. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transfer close to walls is modeled using wall functions

The equations solved by the **Turbulent Flow, k**-ε interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation *k*-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Heat Transfer** interface solves for conservation of energy. A **Fluid** feature is active by default on the entire interface selection. Heat transfer close to walls is modeled using wall functions.

The Nonisothermal Reacting Turbulent Flow, k-ω Interface

The **Nonisothermal Reacting Turbulent Flow, k-ω** ( ) multiphysics interface is used to simulate flow in the turbulent regime, heat transfer, and species transport and in a gas or liquid moving either in a free flow or through the interstices of a porous medium.

This interface requires a license for either the Chemical Reaction Engineering Module, the Battery Design Module, or the Fuel Cell & Electrolyzer Module.

It combines the **Chemistry**, **Transport of Concentrated Species**, **Turbulent Flow, k-ω**, and **Heat Transfer in Fluids** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow, heat transfer and mass transfer. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The multiphysics coupling takes into account the heat of reaction in the fluid and at the surface of a porous catalyst, enthalpy diffusion, and contributing mass fluxes. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transfer close to walls is modeled using wall functions

The equations solved by the **Turbulent Flow, k-ω** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the Wilcox revised k-ω model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Heat Transfer** interface solves for conservation of energy. A **Fluid** feature is active by default on the entire interface selection. Heat transfer close to walls is modeled using wall functions.

The Nonisothermal Reacting Turbulent Flow, SST Interface

The **Nonisothermal Reacting Turbulent Flow, SST** ( ) multiphysics interface is used to simulate flow in the turbulent regime, heat transfer, and species transport and in a gas or liquid moving either in a free flow or through the interstices of a porous medium. This interface requires a license for either the Chemical Reaction Engineering Module, the Battery Design Module, or the Fuel Cell & Electrolyzer Module.

It combines the **Chemistry**, **Transport of Concentrated Species**, **Turbulent Flow, SST**, and **Heat Transfer in Fluids** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow, heat transfer and mass transfer. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The multiphysics coupling takes into account the heat of reaction in the fluid and at the surface of a porous catalyst, enthalpy diffusion, and contributing mass fluxes. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transfer close to walls is modeled using wall functions

The equations solved by the **Turbulent Flow, SST** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the SST model. The SST model is a low-Reynolds number model which means that it resolves the velocity, pressure, and concentrations all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The SST model

depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Heat Transfer** interface solves for conservation of energy. A **Fluid** feature is active by default on the entire interface selection. Heat transfer close to walls is modeled using wall functions.

The Nonisothermal Reacting Turbulent Flow, Low Re k-ε Interface

The **Nonisothermal Reacting Turbulent Flow, Low Re k-ε** ( ) multiphysics interface is used to simulate flow in the turbulent regime, heat transfer, and species transport and in a gas or liquid moving either in a free flow or through the interstices of a porous medium. This interface requires a license for either the Chemical Reaction Engineering Module, the Battery Design Module, or the Fuel Cell & Electrolyzer Module.

It combines the **Chemistry**, **Transport of Concentrated Species**, **Turbulent Flow, Low Re k-ε**, and **Heat Transfer in Fluids** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow, heat transfer and mass transfer. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The multiphysics coupling takes into account the heat of reaction in the fluid and at the surface of a porous catalyst, enthalpy diffusion, and contributing mass fluxes. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transfer close to walls is modeled using wall functions

The equations solved by the **Turbulent Flow, Low Re k-ε** interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the AKN low-Reynolds number k-e model. The low-Reynolds number model resolves the velocity, pressure, and concentrations all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The AKN model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Heat Transfer** interface solves for conservation of energy. A **Fluid** feature is active by default on the entire interface selection. Heat transfer close to walls is modeled using wall functions.

The Reacting Flow Coupling Feature

For the settings of this feature see The Reacting Flow Coupling Feature.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

CHEMISTRY

The available physics features for the Chemistry interface are listed in the section Feature Nodes Available for the Chemistry Interface in the *Chemical Reaction Engineering Module User's Guide*.

LAMINAR FLOW

The available physics features for The Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow in the *CFD Module User's Guide*.

TURBULENT FLOW

The available physics features for a single-phase flow interface using a turbulence model, for example the Turbulent Flow, k-ε interface, is listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow in the *CFD Module User's Guide*.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for the Transport of Concentrated Species interface are listed in the section Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface.

HEAT TRANSFER

The available physics features for the Heat Transfer interface are listed in the section The Heat Transfer Features in the *COMSOL Multiphysics Reference Manual*.

The High Mach Number Reacting Flow Multiphysics Interfaces

The High Mach Number Reacting Flow multiphysics interfaces are predefined interfaces available when licenses for CFD Module and Chemical Reaction Engineering Module are active. They are used to simulate the transport and reaction of species in gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

Selecting the **Laminar Flow** option in the **Chemical Species Transport** > **High Mach Number Reacting Flow** branch of the **Model Wizard**, or an option in the **Chemical Species Transport** > **High Mach Number Reacting Flow** > **Turbulent Flow** branch of the **Model Wizard**, or **Add Physics** windows, the following physics interfaces are added to the Model Builder:

- **High Mach Number Flow, Laminar**, or a turbulent flow equivalent like **High Mach Number Flow, k-ε**.
- **Transport of Concentrated Species**
- **Chemistry**

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature **High Mach Number Reacting Flow**, which predefines and controls the couplings between the separate interfaces in order to facilitate set up of models.

In this section:

- The High Mach Number Reacting Laminar Flow Interface
- The High Mach Number Reacting Turbulent Flow, k-ε Interface
- The High Mach Number Reacting Turbulent Flow, Spalart–Allmaras Interface
- The High Mach Number Reacting Flow Coupling Feature
- Physics Interface Features

The High Mach Number Reacting Laminar Flow Interface

The **High Mach Number Reacting Laminar Flow** ( ) multiphysics interface is used to simulate the transport and reaction of species in gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

It combines the **High Mach Number Flow, Laminar** interface, the **Transport of Concentrated Species** interface and, optionally, the **Chemistry** interface. The **High Mach Number Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport with reactions. The multiphysics coupling takes into account the heat of reaction, enthalpy diffusion, and contributing mass fluxes. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. A **Transport Properties** feature is active by default on the entire interface selection

The equations solved by the **High Mach Number Laminar Flow** interface are the Navier–Stokes equations for conservation of momentum, the continuity equation for conservation of mass and the equation for the conservation of energy. A **Fluid Properties** feature is active by default on the entire interface selection.

The High Mach Number Reacting Turbulent Flow, k-ε Interface

The **High Mach Number Reacting Turbulent Flow, k-ε** ( ) multiphysics interface is used to simulate the transport and reaction of species in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

It combines the **High Mach Number Flow, k-ε** interface, the **Transport of Concentrated Species** interface and, optionally, the **Chemistry** interface. The **High Mach Number Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport with reactions. The multiphysics coupling takes into account the heat of reaction, enthalpy diffusion, and contributing mass fluxes, and applies

turbulence modeling for the mass transport. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transfer close to walls is modeled using wall functions. A **Transport Properties** feature is active by default on the entire interface selection

The equations solved by the **High Mach Number Flow, k-ε** interface are the Navier–Stokes equations for conservation of momentum, the continuity equation for conservation of mass and the equation for the conservation of energy. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions. A **Fluid Properties** feature is active by default on the entire interface selection.

The High Mach Number Reacting Turbulent Flow, Spalart–Allmaras Interface

The **High Mach Number Reacting Turbulent Flow, Spalart–Allmaras** ( ) multiphysics interface is used to simulate the transport and reaction of species in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

It combines the **High Mach Number Flow, Spalart–Allmaras** interface, the **Transport of Concentrated Species** interface and, optionally, the **Chemistry** interface. The **High Mach Number Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport with reactions. The multiphysics coupling takes into account the heat of reaction, enthalpy diffusion, and contributing mass fluxes, and applies turbulence modeling for the mass transport. In addition, the temperature dependency of the chemical properties and reactions are accounted for.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Chemistry** interface defines thermodynamic properties and transport properties of the fluid. Provided that properties of each species have been defined, composition dependent mixture properties such as the heat capacity, the density, and the heat conduction are defined. The **Chemistry** interface also defines reaction rates for species involved in the chemical reactions added to the system.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transfer close to walls is modeled using wall functions. A **Transport Properties** feature is active by default on the entire interface selection

The equations solved by the **High Mach Number Flow, Spalart–Allmaras** interface are the Navier–Stokes equations for conservation of momentum, the continuity equation for conservation of mass and the equation for the conservation of energy. Turbulence effects are modeled using the Spalart–Allmaras one-equation model. The Spalart–Allmaras model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The Spalart–Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation. A **Fluid Properties** feature is active by default on the entire interface selection.

The High Mach Number Reacting Flow Coupling Feature

Use the **High Mach Number Reacting Flow** ( ) multiphysics coupling to simulate mass transport and reactions in a gas mixture where the fluid flow can be dependent on the mixture composition.

The coupling automatically accounts for the heat of reaction, enthalpy diffusion and contributing mass fluxes.

Select a **Fluid Flow** interface and a **Species transport** interface to couple fluid flow with mass transport. **Chemistry** is optional, and if it is selected, the fluid properties are taken from the **Chemistry** interface.

The pressure, velocity, and temperature variables of the **High Mach Number Reacting Flow** coupling node are set to the **Common Model Input** values of the **Default Model Inputs** node on the complementary selection, that is, all domains except those from the **Selection** list. It allows to couple multiple fluid flow or transport of species interfaces with a single heat transfer interface. See Default Model Inputs in the *COMSOL Multiphysics Reference Manual* for details.

DOMAIN LEVEL SYNCHRONIZATION

The **High Mach Number Reacting Flow** coupling synchronizes the features from a High Mach Number Flow interface, a Transport of Concentrated Species interface and, optionally, a Chemistry interface. When the Chemistry interface is not selected, the density in the High Mach Number Flow interface is automatically synchronized to the one defined by the Transport of Concentrated Species interface.

The velocity field used by the Transport of Concentrated Species interface is synchronized to the one computed in the High Mach Number Flow interface.

When a Chemistry interface is selected, the **High Mach Number Reacting Flow** coupling synchronizes the definition of the thermal conductivity, density, heat capacity, enthalpy, molar mass and dynamic viscosity with the other coupled physics interfaces. The reference temperature is taken from the High Mach Number Flow interface.

THE STEFAN VELOCITY

The **High Mach Number Reacting Flow** coupling feature automatically couples mass transfer on boundaries and applies a corresponding velocity contribution for the flow. Prescribing a net mass boundary flux in the **Transport of Concentrated Species** interface, either using a **Flux** or **Mass Fraction** feature, the **High Mach Number Reacting Flow** feature computes The Stefan Velocity and applies this in **Wall** features using the same selection.

TURBULENT MASS TRANSFER

When a turbulence model is used, the **High Mach Number Reacting Flow** coupling applies turbulence modeling for the mass transport in the following manners:

- Turbulent mass transport is added, defined from the turbulent viscosity and a turbulent Schmidt number (for more information, see Turbulent Mass Transport Models).
- Mass transport wall functions. When a turbulence model using wall functions is used for the fluid flow, the **High Mach Number Reacting Flow** coupling automatically adds wall functions for the mass transport on the same boundaries (for more information, see Mass Transport Wall Functions).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `hmnrf1`.

DOMAIN SELECTION

The **High Mach Number Reacting Flow** coupling is automatically defined on the intersection of the selections for the coupled interfaces.

The **Selection** list displays the domains where the coupling feature is active.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow**, **Species transport**, and **Chemistry** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the participating physics interfaces are selected.

You can also select **None** from a list to uncouple the node from a physics interface.

Click the **Go to Source** buttons ( ) to move to the main physics interface node for the selected physics interface.

Click the **Show or Hide Physics Properties Settings** button ( ) to toggle the display of physics properties settings affecting the coupling feature. When a turbulence model is used, turbulent mass transfer is automatically accounted for (see the settings in the **Turbulence** section below). Using **High Mach Number Reacting Flow** coupling, the mass transfer treatment at walls follows that applied for the fluid flow. Therefore the **Wall treatment** setting is also displayed when using a turbulence model. For more information on turbulent mass transfer at walls, see the section Mass Transport Wall Functions in the *CFD Module User's Guide*.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow**, **Species transport**, and **Chemistry** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

MASS TRANSPORT TURBULENCE MODEL

When the fluid flow interface uses a turbulence model, select an option from the **Mass transport turbulence model** list — **Kays–Crawford** or **User-defined turbulent Schmidt number**.

For **User-defined turbulent Schmidt number**, enter a **Turbulent Schmidt number** Sc_T (dimensionless).

The turbulent mass transfer added to the mass fraction equations is defined as, $N_{i,T} = (\mu_T/\mathrm{Sc}_T)\nabla\omega_i$, where, μ_T is the turbulent viscosity defined by the flow interface, and the turbulent Schmidt number, Sc_T, depends on the **Mass transport turbulence model** used.

The **Turbulence model type** used by the fluid flow interface can be displayed by selecting the **Show or Hide Physics Property Settings** button at the right of the **Fluid flow** list.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

HIGH MACH NUMBER FLOW

The available physics features for the High Mach Number Flow interfaces are listed in the section Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for the Transport of Concentrated Species interface are listed in the section Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface.

CHEMISTRY

The available physics features for the Chemistry interface are listed in the section Feature Nodes Available for the Chemistry Interface

The High Mach Number Reacting Flow, Diluted Species Multiphysics Interfaces

The High Mach Number Reacting Flow, Diluted Species multiphysics interfaces are predefined multiphysics interfaces available in the CFD Module. They are used to simulate the transport of dilute species in gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

These physics interfaces support laminar flow and, depending on the licensed products, turbulent flow.

Selecting the **Laminar Flow, Diluted Species** entry in the **Chemical Species Transport** > **High Mach Number Reacting Flow** branch of the **Model Wizard**, or an entry in the **Chemical Species Transport** > **High Mach Number Reacting Flow** > **Turbulent Flow, Diluted Species** branch of the **Model Wizard**, or **Add Physics** windows, the following two physics interfaces are added to the Model Builder:

- **High Mach Number Flow, Laminar**, or a turbulent flow equivalent like **High Mach Number Flow, k-ε**.
- **Transport of Diluted Species**

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature **High Mach Number Reacting Flow, Diluted Species**, which predefines and controls the couplings between the separate interfaces in order to facilitate set up of models.

In this section:

- The High Mach Number Reacting Laminar Flow, Diluted Species Interface
- The High Mach Number Reacting Turbulent Flow, k-ε, Diluted Species Interface
- The High Mach Number Reacting Turbulent Flow, Spalart–Allmaras, Diluted Species Interface
- The High Mach Number Reacting Flow, Diluted Species Coupling Feature
- Physics Interface Features

The High Mach Number Reacting Laminar Flow, Diluted Species Interface

The **High Mach Number Reacting Laminar Flow, Diluted Species** multiphysics interface ( ) is used to simulate the transport of dilute solutes in laminar gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

It combines the **High Mach Number Laminar Flow** and the **Transport of Diluted Species** physics interfaces. The **High Mach Number Reacting Flow, Diluted Species**, which is added automatically, couples the velocity field in the interfaces. The mass transfer solves for the development of one or several solutes dissolved in the gas flow in the transonic and supersonic range.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **High Mach Number Flow** interface are the Navier–Stokes equations for conservation of momentum, the continuity equation for conservation of mass and the equation for the conservation of energy. A **Fluid Properties** feature is active by default on the entire interface selection.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The High Mach Number Reacting Turbulent Flow, k-ε, Diluted Species Interface

The **High Mach Number Reacting Turbulent Flow, k-ε, Diluted Species** multiphysics interface ( ) is used to simulate the transport of dilute solutes in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

It combines the **High Mach Number Flow, k-ε** and the **Transport of Diluted Species** physics interfaces. The **High Mach Number Reacting Flow, Diluted Species**, which is added automatically, couples the velocity field, adds turbulent mixing contributions to the mass transport equations and introduces mass transport turbulence modeling. The mass transfer solves for the development of one or several solutes dissolved in the gas flow in the transonic and supersonic range.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **High Mach Number Flow, k-ε** interface are the Navier–Stokes equations for conservation of momentum, the continuity equation for conservation of mass and the equation for the conservation of energy. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions. A **Fluid Properties** feature is active by default on the entire interface selection.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The High Mach Number Reacting Turbulent Flow, Spalart–Allmaras, Diluted Species Interface

The **High Mach Number Reacting Turbulent Flow, Spalart–Allmaras, Diluted Species** multiphysics interface ( ) is used to simulate the transport of dilute solutes in turbulent gas flows where the velocity magnitude is comparable to the speed of sound in the gas, that is, flows in the transonic and supersonic range.

It combines the **High Mach Number Flow, Spalart–Allmaras** and the **Transport of Diluted Species** physics interfaces. The **High Mach Number Reacting Flow, Diluted Species**, which is added automatically, couples the velocity field, adds turbulent mixing contributions to the mass transport equations and introduces mass transport turbulence modeling. The mass transfer solves for the development of one or several solutes dissolved in the gas flow in the transonic and supersonic range.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **High Mach Number Flow, Spalart–Allmaras** interface are the Navier–Stokes equations for conservation of momentum, the continuity equation for conservation of mass and the equation for the conservation of energy. Turbulence effects are modeled using the Spalart–Allmaras one-equation model. The Spalart–Allmaras model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The Spalart–Allmaras model depends on

the distance to the closest wall. The physics interface therefore includes a wall distance equation. A **Fluid Properties** feature is active by default on the entire interface selection.

The **Transport of Diluted Species** interface solves for an arbitrary number of concentrations. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The High Mach Number Reacting Flow, Diluted Species Coupling Feature

Use the **High Mach Number Reacting Flow, Diluted Species** ( ) multiphysics coupling to simulate mass transport in a gas mixture where the fluid flow contains dissolved dilute species.

Select a **Fluid Flow** interface and a **Species transport** interface to couple fluid flow with mass transport.

DOMAIN LEVEL SYNCHRONIZATION

The **High Mach Number Reacting Flow, Diluted Species** coupling synchronizes the features from a High Mach Number Flow interface and Transport of Diluted Species interface.

The velocity field used by the Transport of Diluted Species interface is synchronized to the one computed in the High Mach Number Flow interface.

THE STEFAN VELOCITY

The **High Mach Number Reacting Flow** coupling feature automatically couples mass transfer on boundaries and applies a corresponding velocity contribution for the flow. Prescribing a net mass boundary flux in the **Transport of Diluted Species** interface, either using a **Flux** or **Mass Fraction** feature, the **High Mach Number Reacting Flow, Diluted Species** feature computes The Stefan Velocity and applies this in **Wall** features using the same selection.

TURBULENT MASS TRANSFER

When a turbulence model is used, the **High Mach Number Reacting Flow, Diluted Species** coupling applies turbulence modeling for the mass transport in the following manners:

- Turbulent mass transport is added, defined from the turbulent viscosity and a turbulent Schmidt number (for more information, see Turbulent Mass Transport Models).
- Mass transport wall functions. When a turbulence model using wall functions is used for the fluid flow, the **High Mach Number Reacting Flow** coupling automatically adds

wall functions for the mass transport on the same boundaries (for more information, see Mass Transport Wall Functions).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `hmnrfd1`.

DOMAIN SELECTION

The **High Mach Number Reacting Flow** coupling is automatically defined on the intersection of the selections for the coupled interfaces.

The **Selection** list displays the domains where the coupling feature is active.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Species transport** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the participating physics interfaces are selected.

You can also select **None** from a list to uncouple the node from a physics interface.

Click the **Go to Source** buttons ( ) to move to the main physics interface node for the selected physics interface.

Click the **Show or Hide Physics Properties Settings** button ( ) to toggle the display of physics properties settings affecting the coupling feature. When a turbulence model is used, turbulent mass transfer is automatically accounted for (see the settings in the **Turbulence** section below). Using **High Mach Number Reacting Flow, Diluted Species** coupling, the mass transfer treatment at walls follows that applied for the fluid flow. Therefore the **Wall treatment** setting is also displayed when using a turbulence model.

For more information on turbulent mass transfer at walls, see the section Mass Transport Wall Functions in the *CFD Module User's Guide*.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** and **Species transport** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

MASS TRANSPORT TURBULENCE MODEL

When the fluid flow interface uses a turbulence model, select an option from the **Mass transport turbulence model** list — **Kays–Crawford** or **User-defined turbulent Schmidt number**.

For **User-defined turbulent Schmidt number**, enter a **Turbulent Schmidt number** Sc_T (dimensionless).

The turbulent mass transfer added to the mass fraction equations is defined as, $N_{i,T} = (\mu_T/\mathrm{Sc}_T)\nabla\omega_i$, where, μ_T is the turbulent viscosity defined by the flow interface, and the turbulent Schmidt number, Sc_T, depends on the **Mass transport turbulence model** used.

The **Turbulence model type** used by the fluid flow interface can be displayed by selecting the **Show or Hide Physics Property Settings** button at the right of the **Fluid flow** list.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

HIGH MACH NUMBER FLOW

The available physics features for the High Mach Number Flow interfaces are listed in the section Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces.

TRANSPORT OF DILUTED SPECIES

The available physics features for the Transport of Diluted Species interface are listed in the section Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface.

The Dispersed Two-Phase Flow with Species Transport Multiphysics Interfaces

Dispersed Two-Phase Flow with Species Transport is a predefined multiphysics interface that couples dispersed two-phase flow with mass transport in both the continuous phase and in the dispersed phase.

Selecting **Laminar Flow** under the **Chemical Species Transport** > **Dispersed Two-Phase Flow with Species Transport** branch of the **Model Wizard** or **Add Physics** windows, a **Mixture Model, Laminar Flow** interface along with a **Continuous Phase Transport of Diluted Species** interface and a **Dispersed Phase Transport of Diluted Species** interface are added to the Model Builder.

In addition, the Multiphysics node is added, including the multiphysics coupling feature **Dispersed Two-Phase Flow, Diluted Species**. The **Dispersed Two-Phase Flow, Diluted Species** feature predefines and controls the couplings between the separate interfaces in order to facilitate easy setup of models.

In this section:

- The Dispersed Two-Phase Laminar Flow with Species Transport Interface
- The Dispersed Two-Phase Turbulent Flow, k-ε, with Species Transport Interface
- The Dispersed Two-Phase Turbulent Flow, k-ω, with Species Transport Interface
- The Dispersed Two-Phase Turbulent Flow, SST, with Species Transport Interface
- The Dispersed Two-Phase Turbulent Flow, Low Re k-ε, with Species Transport Interface
- The Dispersed Two-Phase Flow, Diluted Species Coupling Feature
- Physics Interface Features
- The Continuous Phase Transport of Diluted Species Interface
- The Dispersed Phase Transport of Diluted Species Interface

The Dispersed Two-Phase Laminar Flow with Species Transport Interface

This multiphysics interface ( ) is used to simulate two-phase flow, in the laminar regime, coupled to transport of dilute solutes in each the two fluid phases. It combines the **Mixture Model, Laminar Flow**, the **Continuous Phase Transport of Diluted Species** interface and the **Dispersed Phase Transport of Diluted Species** interface.

The **Dispersed Two-Phase Flow, Diluted Species** multiphysics coupling, which is added automatically, couples the two-phase flow with mass transport. The mass transport interfaces solve for the development of one or several solutes present in the continuous and dispersed fluid phase. The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

- The **Mixture Model, Laminar Flow** interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction.
- The **Continuous Phase Transport of Diluted Species** interface solves for an arbitrary number of solute concentrations present in the continuous phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase.
- The **Dispersed Phase Transport of Diluted Species** interface solves for an arbitrary number of solute concentrations present in the dispersed phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase.

The Dispersed Two-Phase Turbulent Flow, k-ε, with Species Transport Interface

This multiphysics interface ( ) is used to simulate two-phase flow, in the turbulent regime, coupled to transport of dilute solutes in each the two fluid phases.

It combines the **Mixture Model, k**-ε, the **Continuous Phase Transport of Diluted Species** interface and the **Dispersed Phase Transport of Diluted Species** interface. The **Dispersed Two-Phase Flow, Diluted Species** multiphysics coupling, which is added automatically, couples the two-phase flow with mass transport. The mass transport interfaces solve

for the development of one or several solutes present in the continuous and dispersed fluid phase. The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Mixture Model, k-ε** interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the standard two-equation k-ε model with realizability constraints. Flow close to walls is modeled using wall functions.

Continuous Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the continuous phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transfer close to solid walls is modeled using wall functions.

Dispersed Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the dispersed phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transfer close to solid walls is modeled using wall functions.

The Dispersed Two-Phase Turbulent Flow, k-ω, with Species Transport Interface

This multiphysics interface ( ) is used to simulate two-phase flow, in the turbulent regime, coupled to transport of dilute solutes in each the two fluid phases.

It combines the **Mixture Model, k-ω**, the **Continuous Phase Transport of Diluted Species** interface and the **Dispersed Phase Transport of Diluted Species** interface. The **Dispersed Two-Phase Flow, Diluted Species** multiphysics coupling, which is added automatically, couples the two-phase flow with mass transport. The mass transport interfaces solve for the development of one or several solutes present in the continuous and dispersed fluid phase. The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Mixture Model, k-ω** interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Wilcox revised two-equation k-ω model with realizability constraints. The k-ω model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall.

Continuous Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the continuous phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transport close to solid walls follows the setting in the coupled **Mixture Model, k-ω** interface. Using wall functions for the fluid flow, wall functions are applied also for the mass transfer. Using a Low-Reynolds-number wall treatment, the mass transfer conditions are applied directly at the wall.

Dispersed Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the dispersed phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transfer close to solid walls follows the setting in the coupled **Mixture Model, k-ω**. Using wall functions for the fluid flow, wall functions are applied also for the mass transfer. Using a Low-Reynolds-number wall treatment, the mass transfer conditions are applied directly at the wall.

The Dispersed Two-Phase Turbulent Flow, SST, with Species Transport Interface

This multiphysics interface ( ) is used to simulate two-phase flow, in the turbulent regime, coupled to transport of dilute solutes in each the two fluid phases.

It combines the **Mixture Model, SST**, the **Continuous Phase Transport of Diluted Species** interface and the **Dispersed Phase Transport of Diluted Species** interface. The **Dispersed Two-Phase Flow, Diluted Species** multiphysics coupling, which is added automatically, couples the two-phase flow with mass transport. The mass transport interfaces solve for the development of one or several solutes present in the continuous and dispersed fluid phase. The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Mixture Model, SST** interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability constraints. The SST model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

Continuous Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the continuous phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transport close to solid walls follows the setting in the coupled **Mixture Model, SST** interface. Using wall functions for the fluid flow, wall functions are applied also for the mass transfer. Using a Low-Reynolds-number wall treatment, the mass transfer conditions are applied directly at the wall.

Dispersed Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the dispersed phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transport close to solid walls follows the setting in the coupled **Mixture Model, SST** interface. Using wall functions for the fluid flow, wall functions are applied also for the mass transfer. Using a Low-Reynolds-number wall treatment, the mass transfer conditions are applied directly at the wall.

The Dispersed Two-Phase Turbulent Flow, Low Re k-ε, with Species Transport Interface

This multiphysics interface ( ) is used to simulate two-phase flow, in the turbulent regime, coupled to transport of dilute solutes in each the two fluid phases.

It combines the **Mixture Model, Low Re k-ε**, the **Continuous Phase Transport of Diluted Species** interface and the **Dispersed Phase Transport of Diluted Species** interface. The **Dispersed Two-Phase Flow, Diluted Species** multiphysics coupling, which is added

automatically, couples the two-phase flow with mass transport. The mass transport interfaces solve for the development of one or several solutes present in the continuous and dispersed fluid phase. The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The **Mixture Model, Low Re k-ε** interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the AKN two-equation k-ε model with realizability constraints. The AKN model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

Continuous Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the continuous phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transport close to solid walls follows the setting in the coupled **Mixture Model, Low Re k-ε** interface. Using wall functions for the fluid flow, wall functions are applied also for the mass transfer. Using a Low-Reynolds-number wall treatment, the mass transfer conditions are applied directly at the wall.

Dispersed Phase Transport of Diluted Species interface solves for an arbitrary number of solute concentrations present in the dispersed phase. The species equations include transport by convection, and diffusion within the phase, as well as reactions and solute extraction between the continuous and dispersed phase. Mass transport close to solid walls follows the setting in the coupled **Mixture Model, Low Re k-ε** interface. Using wall functions for the fluid flow, wall functions are applied also for the mass transfer. Using a Low-Reynolds-number wall treatment, the mass transfer conditions are applied directly at the wall.

The Dispersed Two-Phase Flow, Diluted Species Coupling Feature

The **Dispersed Two-Phase Flow, Diluted Species** ( ) multiphysics coupling is used to simulate the fluid flow of a liquid containing a dispersed phase, together with mass transport occurring in the continuous phase and the dispersed phase. The coupling feature also support mass transfer (solute extraction) between the phases.

DOMAIN LEVEL SYNCHRONIZATION

The **Dispersed Two-Phase Flow, Diluted Species** coupling synchronizes the features in a Mixture Model interface, with those in the transport interfaces for each of the phases (**Continuous Phase Transport of Diluted Species** and **Dispersed Phase Transport of Diluted Species**). When added, the velocity field and the volume fraction of each of the phases, computed by the Mixture Model interface, is synchronized to the species transport interface for each phase.

SOLUTE EXTRACTION

Extraction is the process where a species is transferred between two immiscible phases due to different relative solubilities in each phase. Physically this transfer process occurs at the phase separating interfaces, the bubble or droplet surfaces in the case of dispersed two phase flow.

Use the checkboxes to select which of the species that can be dissolved in both phases and is subjected to extraction. When multiple species are present in each phase, the species in the two mass transport interfaces are paired by position, from top to bottom, in the **Concentrations** list (in the **Dependent Variables** section when selecting an interface). During extraction, the species in the continuous phase physics interface is transferred into, or from, the corresponding species in the dispersed phase physics interface. The rate at which species is removed from the continuous phase is

$$R_{e,c} = -k_m(K_p c_c - c_d)a_s = -R_{e,d} \tag{8-11}$$

where c_c and c_d are the concentration in the continuous and the dispersed phase respectively. K_p is the partition coefficient determining the phase partitioning at equilibrium, a_s is the dispersed phase specific surface area (m^2/m^3), and k_m is a mass transfer coefficient governing the transport from the bubble or droplet surfaces to the bulk of each phase. Note same source term but with opposite sign is added for the corresponding species in the dispersed phase.

Assuming that the dispersed phase particles are spherical, the specific surface area is computed from the dispersed phase volume fraction ϕ_d and the particle radius r_p in the manner of

$$a_s = \frac{3\phi_d}{r_p} \tag{8-12}$$

When modeling phase transfer with a net mass change between the phases, and a corresponding change in the particle radius, **Solve for interfacial area** can be enabled in

the settings of the coupled Mixture Model interface. In this case the resulting specific area is used in the extraction rate.

TURBULENT MASS TRANSFER

When a turbulence model is used, the **Dispersed Two-Phase Flow, Diluted Species** coupling applies turbulence modeling for species transport interface in the following manners:

- Turbulent mass transport is added, defined from the turbulent viscosity and a turbulent Schmidt number (for more information, see Turbulent Mass Transport Models).
- Mass transport wall functions. When a turbulence model using wall functions is used for the fluid flow, the coupling node automatically adds wall functions for the mass transport on the same boundaries (for more information, see Mass Transport Wall Functions).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `dds1`.

DOMAIN SELECTION

The **Dispersed Two-Phase Flow, Diluted Species** coupling is automatically defined on the intersection of the selections for the coupled interfaces.

The **Selection** list displays the domains where the coupling feature is active.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The lists **Dispersed Two-Phase Flow**, **Continuous phase species**, and **Dispersed phase species** include the applicable physics interfaces of each kind.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (macOS and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Mixture Model, Laminar Flow** is deleted, then the **Dispersed Two-Phase Flow** list defaults to **None** as there is nothing to couple to.

Click the **Go to Source** buttons ( ) to move to the main physics interface node for the selected physics interface.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again using the lists in the **Coupled Interfaces** section. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

TURBULENCE

When the fluid flow interface uses a turbulence model, select an option from the **Mass transport turbulence model** list — **Kays-Crawford**, **High Schmidt Number**, or **User-defined turbulent Schmidt number**.

For **User-defined turbulent Schmidt number**, enter a **Turbulent Schmidt number** Sc_T (dimensionless).

The turbulent mass transfer added to the concentration equations is defined as

$$\mathbf{J}_{T,i} = -\frac{\mu_T}{Sc_T}\nabla c_i$$

where μ_T is the turbulent viscosity defined by the flow interface, and the turbulent Schmidt number, Sc_T, depends on the **Mass transport turbulence model** used.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (macOS or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

MIXTURE MODEL, LAMINAR FLOW

The available physics features for The Mixture Model Laminar Flow interface are listed in the section Domain and Boundary Nodes for the Mixture Model Interfaces.

MIXTURE MODEL, k-ε

The available physics features for the The Mixture Model, k-ε Interface interface are listed in the section Domain and Boundary Nodes for the Mixture Model Interfaces.

MIXTURE MODEL, k-ω

The available physics features for The Mixture Model, k-ω Interface are listed in the section Domain and Boundary Nodes for the Mixture Model Interfaces.

MIXTURE MODEL, SST

The available physics features for The Mixture Model, SST Interface are listed in the section Domain and Boundary Nodes for the Mixture Model Interfaces.

MIXTURE MODEL, LOW RE k-ε

The available physics features for The Mixture Model, Low Re k-ε Interface are listed in the section Domain and Boundary Nodes for the Mixture Model Interfaces.

CONTINUOUS PHASE TRANSPORT OF DILUTED SPECIES AND DISPERSED PHASE TRANSPORT OF DILUTED SPECIES

These interfaces are versions of the Transport of Diluted Species interface. The interfaces extends the functionality by supporting phase specific mass transport. Porous media transport, and migration in an electric field, are however not supported in the interfaces for phase specific mass transport. Apart from Transport Properties, the available features are described in the section Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface.

The Continuous Phase Transport of Diluted Species Interface

The **Continuous Phase Transport of Diluted Species** interface is used to calculate the concentration of one or several a dilute solutes present in a continuous phase in a fluid with multiple immiscible phases. Transport and reactions of the species within the continuous phase can be handled with this interface. The driving forces for transport can be convection by the continuous phase velocity, diffusion by Fick's law, and turbulent diffusion, when the interface is used in The Dispersed Two-Phase Flow, Diluted Species Coupling Feature.

The interface supports simulation of transport 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, c_i, of each species i. It should be noted that the concentration solved for is the total concentration

$$c_i = \phi_c c_{c,i} \tag{8-13}$$

comprised of the phase volume fraction, ϕ_c, and the continuous phase concentration $c_{c,i}$. For each concentration solved for, the interface defines a variable `tds.phs_<concentration>` corresponding to the phase concentration ($c_{c,i}$). This can be used in boundary conditions and reaction rate expressions when the phase concentration is to be prescribed or used.

The Continuous Phase Transport of Diluted Species interface is a version of the Transport of Diluted Species interface. Except for the transport mechanism settings described below, the interface settings are identical to those available in The Transport of Diluted Species Interface.

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the checkboxes available under **Additional transport mechanisms** to control other transport mechanisms.

- By default, the **Convection** checkbox is selected. Clear the checkbox to disable convective transport.
- **Phase specific transport** is enabled by default. When enabled, the **Phase type** can be set to **Continuous** or **Dispersed**. Clear the **Phase specific transport** checkbox to disable the support for a volume fraction and phase specific transport.

The Dispersed Phase Transport of Diluted Species Interface

The **Dispersed Phase Transport of Diluted Species** interface is used to calculate the concentration of one or several a dilute solutes present in a dispersed phase in a fluid with multiple immiscible phases. Transport and reactions of the species within the continuous phase can be handled with this interface. The driving forces for transport can be convection by the dispersed phase velocity, diffusion by Fick's law, and turbulent diffusion, when the interface is used in The Dispersed Two-Phase Flow, Diluted Species Coupling Feature.

The interface supports simulation of species transport in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, c_i, of each species i. It should be noted that the concentration solved for is the total concentration

$$c_i = \phi_{\mathrm{d}} c_{\mathrm{d},i} \tag{8-14}$$

comprised of the phase volume fraction, ϕ_{d}, and the dispersed phase concentration $c_{\mathrm{d},i}$. For each concentration solved for, the interface defines a variable `tds.phs_<concentration>` corresponding to the phase concentration ($c_{\mathrm{d},i}$). This can be used in boundary conditions and reaction rate expressions when the phase concentration is to be prescribed or used.

The Dispersed Phase Transport of Diluted Species interface is a version of the Transport of Diluted Species interface. Except for the transport mechanism settings described below, the interface settings are identical to those available in The Transport of Diluted Species Interface.

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the checkboxes available under **Additional transport mechanisms** to control other transport mechanisms.

- By default, the **Convection** checkbox is selected. Clear the checkbox to disable convective transport.
- **Phase specific transport** is enabled by default. When enabled, the **Phase type** can be set to **Continuous** or **Dispersed**. Clear the **Phase specific transport** checkbox to disable the support for a volume fraction and phase specific transport.

Transport Properties

Use this node to define the volume fraction, the convective velocity, and the diffusion coefficient to use for the phase specific transport in a Continuous Phase Transport of Diluted Species interface or a Dispersed Phase Transport of Diluted Species interface.

Conservation of mass of a species i in an immiscible fluid phase is formulated as

$$\frac{\partial \phi \rho_i}{\partial t} + \nabla \cdot (\phi \rho_i \mathbf{u}) = \nabla \cdot [D_i \nabla (\phi \rho_i)] + R_{\mathrm{m},i} \tag{8-15}$$

where ϕ is the phase volume fraction, ρ_i the species density, and $\mathbf{u}$ the (mass averaged) velocity of the phase, D_i is the diffusion coefficient, and $R_{\mathrm{m},i}$ is the species mass source. Using the species density definition $\rho_i = c_{\mathrm{p},i} M_i$, where $c_{\mathrm{p},i}$ is the species phase concentration, and diving by the molar mass M_i, the conservation equation becomes

$$\frac{\partial \phi c_{\mathrm{p},i}}{\partial t} + \nabla \cdot (\phi c_{\mathrm{p},i} \mathbf{u}) = \nabla \cdot [D_i \nabla (\phi c_{\mathrm{p},i})] + R_i \tag{8-16}$$

Choosing to solve for the total concentration $c_i = \phi c_{\mathrm{p},i}$, the equation is

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (c_i \mathbf{u}) = \nabla \cdot (D_i \nabla c_i) + R_i \tag{8-17}$$

The following equations are solved for the total species concentration in the continuous and the dispersed phase respectively

$$\frac{\partial c_{\mathrm{c},i}}{\partial t} + \nabla \cdot (c_{\mathrm{c},i} \mathbf{u}_{\mathrm{c}}) = \nabla \cdot [(D_{\mathrm{c},i} + D_{\mathrm{T},i}) \nabla c_{\mathrm{c},i}] + R_{\mathrm{c},i} \tag{8-18}$$

$$\frac{\partial c_{\mathrm{d},i}}{\partial t} + \nabla \cdot (c_{\mathrm{d},i} \mathbf{u}_{\mathrm{d}}) = \nabla \cdot [(D_{\mathrm{d},i} + D_{\mathrm{T},i}) \nabla c_{\mathrm{d},i}] + R_{\mathrm{d},i} \tag{8-19}$$

Here $D_{\mathrm{T},i}$ is a turbulent dispersion coefficient accounting for the enhanced transport in turbulent flow. It is added by the Dispersed Two-Phase, Diluted Species coupling feature when the Mixture Model interface is using a turbulence model.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

VOLUME FRACTION

Specify the phase volume fraction. Select the source of the **Volume fraction, continuous phase** or the source of the **Volume fraction, dispersed phase**. When using a Dispersed Two-Phase Flow, Diluted Species coupling feature, the volume fraction is automatically coupled to the one computed by the Mixture Model interface in the same coupling.

CONVECTION

If transport by convection is active, the velocity field of the phase in question needs to be specified. Select the source of the **Velocity field, continuous phase** or the source of the **Velocity field, dispersed phase**. When using a Dispersed Two-Phase Flow, Diluted Species coupling feature, the velocity is automatically coupled to the one computed by the Mixture Model interface in the same coupling.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the respective phase.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Fluid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Fluid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Fluid diffusion coefficient** list.

For **User defined**, enter a value or expression for the **Fluid diffusion coefficient** D_c of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

Theory for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution of chemical species transported by diffusion and convection. The physics interface assumes that all species present are dilute; that is, that their concentration is low compared to a solvent fluid or solid. As a rule of thumb, a mixture containing several species can be considered dilute when the concentration of the solvent is more than 90 mol%. Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent.

When studying mixtures that are not dilute, the mixture and transport properties depend on the composition, and a different physics interface is recommended. See The Transport of Concentrated Species Interface in the *Chemical Reaction Engineering Module User's Guide* for more information.

Fick's law governs the diffusion of the solutes, dilute mixtures, or solutions, while the phenomenon of ionic migration is sometimes referred to as *electrokinetic flow*. The Transport of Diluted Species interface supports the simulations of chemical species transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D.

In this section:

- Adding Transport Through Migration
- Material Balance Formulation
- Crosswind Diffusion
- Danckwerts Inflow Boundary Condition
- Equilibrium Reaction Theory
- Mass Balance Equation
- Mass Sources for Species Transport
- Solving a Diffusion Equation Only
- Supporting Electrolytes
- References

Note: Some features explained in this section require certain add-on modules. For details see https://www.comsol.com/products/specifications/

The section also includes the theory for The Transport of Diluted Species in Porous Media Interface:

- Adsorption
- Convection in Porous Media
- Diffusion in Porous Media
- Dispersion
- Mass Balance Equation for Transport of Diluted Species in Porous Media
- Mass Transport in Fractures
- Reactions

Mass Balance Equation

The default node attributed to the Transport of Diluted Species interface models chemical species transport through diffusion and convection and solves the mass conservation equation for one or more chemical species i:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i \tag{8-20}$$

Equation 8-20 in its form above includes the transport mechanisms diffusion and convection. If *Migration in Electric Field* is activated (only available in some add-on products), the migration mechanism will be added to the equation as well. See more details in the section Adding Transport Through Migration.

- c_i is the concentration of the species (SI unit: mol/m^3)
- D_i denotes the diffusion coefficient (SI unit: m^2/s)
- R_i is a reaction rate expression for the species (SI unit: mol/(m^3·s))
- $\mathbf{u}$ is the mass averaged velocity vector (SI unit: m/s)
- $\mathbf{J}_i$ is the mass flux diffusive flux vector (SI unit: mol/(m^2·s))

The mass flux relative to the mass averaged velocity, $\mathbf{J}_i$ (SI unit: mol/(m^2·s)), is associated with the mass balance equation above and used in boundary conditions and flux computations. The Transport of Diluted Species interface always includes mass transport due to molecular diffusion. In this case the mass flux $\mathbf{J}_i$ defines the diffusive flux vector

$$\mathbf{J}_i = -D\nabla c_i \tag{8-21}$$

An input field for the diffusion coefficient is available.

When *Migration in Electric Fields* is activated, the migration term is also added to the diffusive flux vector as shown in the section Adding Transport Through Migration.

The third term on the left side of Equation 8-20 describes the convective transport due to a velocity field **u**. This field can be expressed analytically or obtained from coupling the physics interface to one that solves for fluid flow, such as *Laminar Flow*. Note that all fluid flow interfaces solve for the mass averaged velocity.

On the right-hand side of the mass balance equation (Equation 8-20), R_i represents a source or sink term, typically due to a chemical reaction or desorption on a porous matrix. To specify R_i, another node must be added to the Transport of Diluted Species interface — the **Reaction** node for example, which includes an input field for specifying a reaction expression using the variable names of all participating species.

Equilibrium Reaction Theory

The feature Equilibrium Reaction is described in this section. A chemical equilibrium reaction system is defined by the stoichiometry of the reaction and the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition).

The kinetics of the reaction is so fast that the equilibrium condition is fulfilled at all times in all space coordinates.

The equilibrium condition is commonly based on the stoichiometric coefficients, ν_i (dimensionless), of the reaction; the species activities of the reacting species a_i (dimensionless); and an equilibrium constant, K_{eq} (1) according to

$$K_{\mathrm{eq}} = \frac{\prod_{i \in \text{ products}} a_i^{\nu_i}}{\prod_{i \in \text{ reactants}} a_i^{-\nu_i}}$$

where the species activities are defined as

$$a_i = \gamma_{c,i} \frac{c_i}{c_{\mathrm{a0}}}$$

where c_{a0} (SI unit: mol/m^3) is the standard molarity, and $\gamma_{c,i}$ (dimensionless) an activity coefficient.

Defining the stoichiometric coefficients positive for products and negative for reactants, the above equilibrium condition can also be written

$$K_{\mathrm{eq}} = \prod_i a_i^{\nu_i}$$

The Equilibrium Reaction node solves for a reaction rate so that the equilibrium condition is always fulfilled in the domain. It is available for the Chemical Reaction Engineering Module; Battery Design Module; Corrosion Module; Electrochemistry Module; Electrodeposition Module; and Fuel Cell & Electrolyzer Module.

$\gamma_{c,i}$ is set to unity when the Equilibrium constant is selected in the Settings window. For nonunity activity coefficients, a user-defined equilibrium condition can be used.

EQUILIBRIUM REACTIONS AND INFLOW BOUNDARY CONDITIONS

Contradictory constraints arise if the boundary conditions for concentrations or activities are set so that the domain equilibrium condition is not fulfilled. Special treatment is therefore needed at Inflow boundaries, where the concentrations are set for all species in the mass transport interfaces.

One way of avoiding competing constraints on an inflow boundary is to add an additional reaction coordinate degree of freedom, solved for to create a set of modified inflow concentrations that fulfill the domain equilibrium condition. The reaction coordinate gives rise to a concentration shift, which is the offset to the inflow concentrations provided by the user. The shift for each species obeys the stoichiometry of the reaction and the equilibrium expression. The modified inflow concentrations are then used in the boundary conditions for the domain mass transport equations. The resulting modified inflow concentrations can be seen as the stationary solution for a batch reactor with the user inflow concentrations as initial concentrations. In addition, the domain reaction rate degree of freedom of the equilibrium reaction is constrained to zero on all Inflow boundaries.

EQUILIBRIUM REACTIONS AND CONCENTRATION BOUNDARY CONDITIONS

No special treatment is made with regards to input concentration values of the Concentration boundary node. Using this feature, you can explicitly set one or a set of concentrations, and the equilibrium condition acts on the rest of the concentrations.

However, there is no solution to the problem if more concentrations than the number of species minus the number of equilibrium reactions are set using this feature.

EQUILIBRIUM REACTIONS AND TIME-DEPENDENT SIMULATIONS

Spurious oscillations may occur in a time-dependent problem if the initial conditions do not fulfill the equilibrium condition. Since equilibrium reactions are assumed to be infinitely fast, the solution is to initialize the problem using an additional study step, solving for a stationary problem with all nonequilibrium reaction rates set to zero. Manual scaling of the reaction rate dependent variables is needed in this study step.

Material Balance Formulation

The default node attributed to The Transport of Diluted Species Interface assumes chemical species transport through diffusion and convection (depending on the modules licensed, a checkbox to activate migration is available) and implements the mass balance equation in Equation 8-20.

Two formulations of the mass balance are available, these are referred to as the nonconservative and conservative form:

$$\text{nonconservative: } \frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c = R \tag{8-22}$$

$$\text{conservative: } \frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J}_i + \nabla \cdot (c\mathbf{u}) = R \tag{8-23}$$

In these equations $\mathbf{J}_i$ is the diffusive flux vector, $\mathbf{u}$ is the solvent velocity field, and R is a production or consumption rate expression. The nonconservative is often more numerically robust, and therefore chosen by default for the interface. This formulation however disregards density changes in the fluid. This can be seen by expanding the conservative convection term using the chain rule. One of the resulting terms, $c\nabla\cdot\mathbf{u}$, equals zero for an incompressible fluid which results in the nonconservative form. To switch between the two formulations, click the **Show** button ( ) and select **Advanced Physics Options**.

Solving a Diffusion Equation Only

Remove the convection term from Equation 8-22 and Equation 8-23 by clearing the Convection checkbox in the Transport Mechanisms section for The Transport of Diluted Species Interface. The equation then becomes

$$\frac{\partial c}{\partial t} = \nabla \cdot \mathbf{J}_i + R$$

Mass Sources for Species Transport

Note: The features below are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

There are two types of mass sources in the Transport of Diluted Species interface: point sources and line sources.

POINT SOURCE

A point source is theoretically formed by assuming a mass injection/ejection, Q_c (SI unit: mol/(m^3·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_{p,c}$ (SI unit: mol/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} Q_c = \dot{q}_{p,c} \tag{8-24}$$

An alternative way to form a point source is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant results in the same point source. For this alternative approach, effects resulting from the physical object's volume need to be neglected.

The weak contribution

$$\dot{q}_{p,c}\text{test}(c)$$

is added at a point in the geometry. As can be seen from Equation 8-24, Q_c must tend to plus or minus infinity as δV tends to zero. This means that in theory the concentration also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 8-24 corresponds to a finite concentration at a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region but also a more extreme concentration value. It is important not to mesh too finely around a point source since this can result in unphysical concentration values. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $Q_{l,c}$ (SI unit: mol/(m^3·s)), located within a tube with cross section δS and then letting δS tend to zero while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_{l,c}$ (SI unit: mol/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} Q_{l,c} = q_{l,c} \tag{8-25}$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects resulting from the physical object's volume are neglected.

The weak contribution

$$q_{l,c}\,\text{test}(c)$$

is added on lines in 3D or at points in 2D (which represent cut-through views of lines). Line sources can also be added on the axisymmetry line in 2D axisymmetry components. It cannot, however, be added on geometrical lines in 2D since those represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

For feature node information, see Line Mass Source and Point Mass Source.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, these shared physics nodes are renamed as follows:

- The **Line Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).
- The **Point Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

Adding Transport Through Migration

Note: Migration is only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

In addition to transport due to convection and diffusion, the Transport of Diluted Species interface supports ionic species transport by *migration*. This is done by selecting the Migration in Electric Field checkbox under the Transport Mechanisms section for the physics interface. The mass balance then becomes:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V + c_i \mathbf{u}) = R_i \tag{8-26}$$

where

- c_i (SI unit: mol/ m^3) denotes the concentration of species i
- D_i (SI unit: m^2/s) is the diffusion coefficient of species i
- $\mathbf{u}$ (SI unit: m/s) is the fluid velocity
- F (SI unit: A·s/mol) refers to Faraday's constant
- V (SI unit: V) denotes the electric potential
- z_i (dimensionless) is the charge number of the ionic species, and
- $u_{\mathrm{m},i}$ (SI unit: mol·s/kg) is its ionic mobility

In this case the diffusive flux vector is

$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V$$

The velocity, $\mathbf{u}$, can be a computed fluid velocity field from a Fluid Flow interface or a specified function of the spatial variables x, y, and z. The potential can be provided by an expression or by coupling the system of equations to a current balance, such as the Electrostatics interface. Sometimes it is assumed to be a supporting electrolyte present, which simplifies the transport equations. In that case, the modeled charged species concentration is very low compared to other ions dissolved in the solution. Thus, the species concentration does not influence the solution's conductivity and the net charge within the fluid.

The Nernst–Einstein relation can in many cases be used for relating the species mobility to the species diffusivity according to

$$u_{m,i} = \frac{D_i}{RT}$$

where R (SI unit: J/(mol·K)) is the molar gas constant and T (SI unit: K) is the temperature.

Note: In the *Nernst–Planck Equations* interface, the ionic species contribute to the charge transfer in the solution. It includes an *electroneutrality condition* and also computes the electric potential field in the electrolyte. For more information, see Theory for the Nernst–Planck Equations Interface. This interface is included in the Chemical Reaction Engineering Module.

Supporting Electrolytes

In *electrolyte* solutions, a salt can be added to provide a high electrolyte conductivity and decrease the ohmic losses in a cell. These solutions are often called *supporting electrolytes*, buffer solutions, or carrier electrolytes. The added species, a negative and a positive ion pair, predominates over all other species. Therefore, the supporting electrolyte species can be assumed to dominate the current transport in the solution. In addition, the predominant supporting ions are usually selected so that they do not react at the electrode surfaces since the high conductivity should be kept through the process, that is, they should not be electroactive species. This also means that the concentration gradients of the predominant species in a supporting electrolyte are usually negligible.

Modeling and solving for a supporting electrolyte in the *Electrostatics* or *Secondary Current Distribution* interfaces will give a potential distribution that drives the migration in the Transport of Diluted Species Interface.

The current density vector is proportional to the sum of all species fluxes as expressed by Faraday's law:

$$\mathbf{i} = F\sum_i z_i \mathbf{N}_i$$

The electroneutrality condition ensures that there is always a zero net charge at any position in a dilute solution. Intuitively, this means that it is impossible to create a current by manually pumping positive ions in one direction and negative ions in the other. Therefore, the convective term is canceled out to yield the following expression for the electrolyte current density, where j denotes the supporting species:

$$\mathbf{i} = F\sum_j -z_j^2 u_{\mathrm{m},j} F c_j \nabla\phi \tag{8-27}$$

Equation 8-27 is simply Ohm's law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa\nabla\phi \tag{8-28}$$

where κ is the conductivity of the supporting electrolyte. A current balance gives the current and potential density in the cell

$$\nabla \cdot \mathbf{i} = 0$$

which, in combination with Equation 8-28, yields:

$$\nabla \cdot (-\kappa\nabla\phi) = 0 \tag{8-29}$$

Equation 8-29 can be easily solved using the Electrostatics or Secondary Current Distribution interface and, when coupled to the Transport in Diluted Species interface, the potential distribution shows up in the migration term.

Crosswind Diffusion

Transport of diluted species applications can often result in models with a very high cell Péclet number — that is, systems where convection or migration dominates over diffusion. Streamline diffusion and crosswind diffusion are of paramount importance to obtain physically reasonable results. The Transport of Diluted Species interface

provides two crosswind diffusion options using different formulations. Observe that crosswind diffusion makes the equation system nonlinear even if the transport equation is linear.

DO CARMO AND GALEÃO

This is the formulation described in Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*. The method reduces over- and undershoots to a minimum, even for anisotropic meshes.

In some cases, the resulting nonlinear equation system can be difficult to converge. This can happen when the cell Péclet number is very high and the model contains many thin layers, such as contact discontinuities. You then have three options:

- Refine the mesh, especially in regions with thin layers.
- Use a nonlinear solver with a constant damping factor less than one.
- Switch to the Codina crosswind formulation.

CODINA

The Codina formulation is described in Ref. 1. It adds diffusion strictly in the direction orthogonal to the streamline direction. Compared to the do Carmo and Galeão formulation, the Codina formulation adds less diffusion but is not as efficient at reducing over- and undershoots. It also does not work as well for anisotropic meshes. The advantage is that the resulting nonlinear system is easier to converge and that underresolved gradients are less smeared out.

Danckwerts Inflow Boundary Condition

Constraining the composition to fixed values at an inlet to a reactor may sometimes result in issues with unreasonably high reaction rates or singularities at the inlet boundary. These problems may many times be mitigated by using a flux boundary condition instead, based on the upstream concentrations and the fluid velocity at the boundary. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet conditions for domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an upstream concentration $c_{i,0}$, the Danckwerts inflow boundary condition prescribed the total flux as

$$\mathbf{n} \cdot (\mathbf{J}_i + \mathbf{u}c_i) = \mathbf{n} \cdot (\mathbf{u}c_{i,0}) \tag{8-30}$$

Mass Balance Equation for Transport of Diluted Species in Porous Media

VARIABLY SATURATED POROUS MEDIA

The following equations for the molar concentrations, c_i, describe the transport of solutes in a variably saturated porous medium for the most general case, when the pore space is primarily filled with liquid but also contain pockets or immobile gas:

$$\frac{\partial}{\partial t}(\theta_l c_i) + \frac{\partial}{\partial t}(\rho c_{P,i}) + \frac{\partial}{\partial t}(\theta_g c_{G,i}) + \mathbf{u} \cdot \nabla c_i = \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_i] + R_i + S_i \tag{8-31}$$

On the left-hand side of Equation 8-31, the first three terms correspond to the accumulation of species within the liquid, solid, and gas phases, while the last term describes the convection due to the velocity field $\mathbf{u}$ (SI unit: m/s).

In Equation 8-31 c_i denotes the concentration of species i in the liquid (SI unit: mol/m^3), $c_{P,i}$ the amount adsorbed to solid particles (moles per unit dry weight of the solid), and $c_{G,i}$ the concentration of species i in the gas phase.

The equation balances the mass transport throughout the porous medium using the porosity ε_p, the liquid volume fraction θ_l; the dry bulk density, $\rho = (1 - \varepsilon_p)\rho_s$, and the solid phase density ρ_s.

For saturated porous media, the liquid volume fraction θ_l is equal to the porosity ε_p, but for unsaturated porous media, they are related by the saturation s as $\theta_l = \varepsilon_p s$. The resulting gas volume fraction in the case of an unsaturated porous medium is

$$\theta_g = \varepsilon_p - \theta_l = (1 - s)\varepsilon_p$$

On the right-hand side of Equation 8-31, the first term introduces the spreading of species due to mechanical mixing resulting from the porous media (dispersion), as well as from diffusion and volatilization to the gas phase. The dispersion tensor is denoted D_D (SI unit: m^2/s) and the effective diffusion by D_e (SI unit: m^2/s).

The last two terms on the right-hand side of Equation 8-31 describe production or consumption of the species; R_i is a reaction rate expression which can account for reactions in the liquid, solid, or gas phase, and S_i is an arbitrary source term, for example due to a fluid flow source or sink.

Adsorption

The time evolution of the adsorption, the solute transport to or from the solid phase, is defined by assuming that the amount of solute adsorbed to the solid, $c_{\mathrm{P},i}$, is a function of the concentration in the fluid c_i. This implies that the solute concentration in the liquid and solid phase are in instant equilibrium. The adsorption term can be expanded to give

$$\frac{\partial}{\partial t}(\rho c_{\mathrm{P},i}) = \rho\frac{\partial c_{\mathrm{P},i}}{\partial c_i}\frac{\partial c_i}{\partial t} - c_{\mathrm{P},i}\rho_s\frac{\partial \varepsilon_p}{\partial t} = \rho K_{\mathrm{P},i}\frac{\partial c_i}{\partial t} - c_{\mathrm{P},i}\rho_s\frac{\partial \varepsilon_p}{\partial t} \tag{8-32}$$

where $K_{\mathrm{P},i} = \partial c_{\mathrm{P},i}/\partial c_i$ is the adsorption isotherm.

Volatilization

Volatilization is the process where a solute species in the liquid is transported to the gas phase due to vaporization. Assuming that the amount of solute in the gas phase, $c_{\mathrm{G},i}$, is a linear function of the liquid phase concentration, the volatilization term is defined as

$$\frac{\partial}{\partial t}\theta_g c_{\mathrm{G},i} = \theta_g\frac{\partial c_{\mathrm{G},i}}{\partial c_i}\frac{\partial c_i}{\partial t} + k_{\mathrm{G},i}c_i\frac{\partial \theta_g}{\partial t} = \theta_g k_{\mathrm{G},i}\frac{\partial c_i}{\partial t} + k_{\mathrm{G},i}c_i\frac{\partial \theta_g}{\partial t} \tag{8-33}$$

where $k_{\mathrm{G},i} = \partial c_{\mathrm{G},i}/\partial c_i$ is the linear volatilization.

SATURATED POROUS MEDIA

In the case of transport in a saturated porous medium, $\theta_l = \varepsilon_p$, and the governing equations are

$$\frac{\partial}{\partial t}(\varepsilon_p c_i) + \frac{\partial}{\partial t}(\rho c_{\mathrm{P},i}) + \mathbf{u}\cdot\nabla c_i = \nabla\cdot[(D_{\mathrm{D},i} + D_{\mathrm{e},i})\nabla c_i] + R_i + S_i \tag{8-34}$$

Convection in Porous Media

Convection (also called advection) describes the movement of a species, such as a pollutant, with the bulk fluid velocity. The velocity field **u** corresponds to a superficial volume average over a unit volume of the porous medium, including both pores and matrix. This velocity is sometimes called *Darcy velocity*, and defined as volume flow

rates per unit cross section of the medium. This definition makes the velocity field continuous across the boundaries between porous regions and regions with free flow.

The velocity field to be used in the Model Inputs section on the physics interface can, for example, be prescribed using the velocity field from a Darcy's Law or a Brinkman Equations interface.

The average linear fluid velocities $\mathbf{u}_a$, provides an estimate of the fluid velocity within the pores:

$$\mathbf{u}_a = \frac{\mathbf{u}}{\varepsilon_p} \quad \text{Saturated}$$

$$\mathbf{u}_a = \frac{\mathbf{u}}{\theta_l} \quad \text{Unsaturated}$$

where ε_p is the porosity and $\theta_l = s\varepsilon_p$ the liquid volume fraction, and s the saturation, a dimensionless number between 0 and 1.

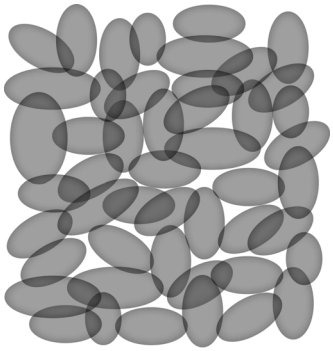

Figure 8-3: A block of a porous medium consisting of solids and the pore space between the solid grains. The average linear velocity describes how fast the fluid moves within the pores. The Darcy velocity attributes this flow over the entire fluid-solid face.

MATERIAL BALANCE FORMULATION

The Transport of Diluted Species interface in porous media includes two formulations of the material balance. The conservative formulation of the species equations in Equation 8-31 is written as:

$$\frac{\partial}{\partial t}(\theta_l c_i) + \frac{\partial}{\partial t}(\rho c_{P,i}) + \frac{\partial}{\partial t}(\theta_g c_{G,i}) + \nabla \cdot \mathbf{u} c_i = \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_i] + R_i + S_i \quad (8\text{-}35)$$

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c_i \nabla \cdot \mathbf{u}$, would equal zero for an incompressible fluid and would result in the nonconservative formulation described in Equation 8-31.

When using the nonconservative formulation, which is the default, the fluid is assumed incompressible and divergence free: $\nabla \cdot \mathbf{u} = 0$. The nonconservative formulation improves the stability of systems coupled to a momentum equation (fluid flow equation).

To switch between the two formulations, click the **Show** button ( ) and select **Advanced Physics Options**. In the section **Advanced Settings** select either **Nonconservative** (the default) or **Conservative**. The conservative formulation should be used for compressible flow.

Diffusion in Porous Media

The effective diffusion in porous media, D_e, depends on the structure of the porous material and the phases involved. Dependent on whether the transport of diluted species occurs in free flow or in saturated or unsaturated porous media, the effective diffusivity is defined as:

$$D_e = D_F \quad \text{Free Flow}$$

$$D_e = \frac{\varepsilon_p}{\tau_L} D_L \quad \text{Saturated Porous Media}$$

$$D_e = \frac{\theta_l}{\tau_L} D_L \quad \text{Unsaturated Porous Media}$$

$$D_e = \frac{\theta_l}{\tau_L} D_L + \frac{\theta_g}{\tau_G} k_G D_G \quad \text{Unsaturated with Volatilization}$$

Here D_F, D_L, and D_G are the single-phase diffusion coefficients for the species diluted in a fluid, a pure liquid, and a gas phase, respectively (SI unit: m^2/s), and τ_F, τ_L, and τ_G are the corresponding tortuosity factors (dimensionless).

The tortuosity factor accounts for the reduced diffusivity due to the fact that the solid grains impede Brownian motion. The interface provides predefined expressions to

compute the tortuosity factors in partially saturated porous media according to the Millington and Quirk model (Ref. 3):

$$\tau_L = \theta_l^{-7/3}\varepsilon_p^{\,2},\ \tau_G = \theta_g^{-7/3}\varepsilon_p^{\,2}$$

and Bruggeman model

$$\tau_L = \theta_l^{-5/2}\varepsilon_p^{\,2},\ \tau_G = \theta_g^{-5/2}\varepsilon_p^{\,2}$$

For saturated porous media $\theta_l = \varepsilon_p$. The fluid tortuosity for the Millington and Quirk model is

$$\tau_L = \varepsilon_p^{-1/3}$$

and for the Bruggeman model the tortuosity is defined as

$$\tau_L = \varepsilon_p^{-1/2}$$

User defined expressions for the tortuosity factor can also be applied.

Dispersion

The contribution of dispersion to the mixing of species typically overshadows the contribution from molecular diffusion, except when the fluid velocity is very low.

The spreading of mass, as a fluid travel through a porous medium is caused by several contributing effects. Local variations in fluid velocity lead to mechanical mixing referred to as dispersion occurs because the fluid in the pore space flows around solid particles, so the velocity field varies within pore channels. The spreading in the direction parallel to the flow, or *longitudinal dispersivity*, typically exceeds the *transverse dispersivity* from up to an order of magnitude. Being driven by the concentration gradient alone, molecular diffusion rate is low relative to the mechanical dispersion, except at very low fluid velocities.

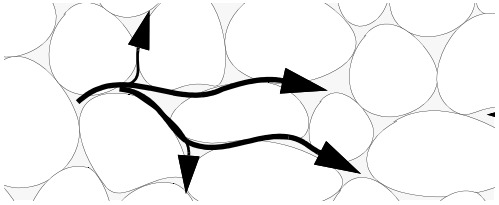

Figure 8-4: Spreading of fluid around solid particles in a porous medium.

The dispersion is controlled through the dispersion tensor D_{D}. The tensor components can either be given by user-defined values or expressions or derived from the directional dispersivities.

Using the longitudinal and transverse dispersivities in 2D, the dispersivity tensor components are (Ref. 5):

$$D_{\mathrm{D}ii} = \alpha_{\mathrm{L}}\frac{u_i^2}{|\mathbf{u}|} + \alpha_{\mathrm{T}}\frac{u_j^2}{|\mathbf{u}|}$$

$$D_{\mathrm{D}ij} = D_{\mathrm{D}ji} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}})\frac{u_i u_j}{|\mathbf{u}|}$$

In these equations, $D_{\mathrm{D}ii}$ (SI unit: m^2/s) are the principal components of the dispersivity tensor, and $D_{\mathrm{D}ji}$ and $D_{\mathrm{D}ji}$ are the cross terms. The parameters α_{L} and α_{T} (SI unit: m) specify the longitudinal and transverse dispersivities; and u_i (SI unit: m/s) stands for the velocity field components.

In order to facilitate modeling of stratified porous media in 3D, the tensor formulation by Burnett and Frind (Ref. 4) can be used. Consider a transverse isotropic media, where the strata are piled up in the z direction, the dispersivity tensor components are:

$$
\begin{aligned}
D_{\mathrm{L}xx} &= \alpha_1\frac{u^2}{|\mathbf{u}|} + \alpha_2\frac{v^2}{|\mathbf{u}|} + \alpha_3\frac{w^2}{|\mathbf{u}|}\\
D_{\mathrm{L}yy} &= \alpha_1\frac{v^2}{|\mathbf{u}|} + \alpha_2\frac{u^2}{|\mathbf{u}|} + \alpha_3\frac{w^2}{|\mathbf{u}|}\\
D_{\mathrm{L}zz} &= \alpha_1\frac{w^2}{|\mathbf{u}|} + \alpha_3\frac{u^2}{|\mathbf{u}|} + \alpha_3\frac{v^2}{|\mathbf{u}|}\\
D_{\mathrm{L}xy} &= D_{\mathrm{L}yx} = (\alpha_1 - \alpha_2)\frac{uv}{|\mathbf{u}|}\\
D_{\mathrm{L}xz} &= D_{\mathrm{L}zx} = (\alpha_1 - \alpha_3)\frac{uw}{|\mathbf{u}|}\\
D_{\mathrm{L}yz} &= D_{\mathrm{L}zy} = (\alpha_1 - \alpha_3)\frac{vw}{|\mathbf{u}|}
\end{aligned}
\tag{8-36}
$$

In Equation 8-36 the fluid velocities u, v, and w correspond to the components of the velocity field $\mathbf{u}$ in the x, y, and z directions, respectively, and α_1 (SI unit: m) is the longitudinal dispersivity. If z is the vertical axis, α_2 and α_3 are the dispersivities in the transverse horizontal and transverse vertical directions, respectively (SI unit: m). Setting $\alpha_2 = \alpha_3$ gives the expressions for isotropic media shown in Bear (Ref. 5 and Ref. 6).

Adsorption

As species travel through a porous medium they typically attach to (adsorb), and detach (desorb) from the solid phase, which slows chemical transport through the porous medium. Adsorption and desorption respectively reduces or increases species concentrations in the fluid. The adsorption properties vary between chemicals, so a plume containing multiple species can separate into components (Ref. 7). The Adsorption feature includes four predefined and one user-defined relationships to predict the solid concentrations, $c_{\mathrm{P}i}$ from the concentration in the liquid phase, c_i:

$$c_P = c_{Pmax}\frac{K_L c}{1+K_L c} \quad \text{Langmuir}$$

$$c_P = K_F\left(\frac{c}{c_{ref}}\right)^N \quad \text{Freundlich}$$

$$c_P = c_{Pmax}\frac{b_T c}{(1+(b_T c)^{N_T})^{1/N_T}} \quad \text{Toth} \qquad (8\text{-}37)$$

$$c_P = \frac{K_B c_0 c}{(c_S - c)\left(1+(K_B-1)\frac{c}{c_S}\right)} \quad \text{BET}$$

The above equations contains the following parameters:

- Freundlich (Ref. 8)
  - Freundlich constant K_F (SI unit:·mol/kg), Freundlich exponent N_F (dimensionless), and reference concentration c_{ref} (SI unit: mol/m^3).
- Langmuir (Ref. 9)
  - Langmuir constant K_L (SI unit: m^3/mol), and adsorption maximum c_{Pmax} (SI unit: mol/kg).
- Toth (Ref. 10)
  - Toth constant b_T (SI unit: m^3/mol), Toth exponent N_T (dimensionless), and adsorption maximum c_{Pmax} (SI unit: mol/kg).
- BET (Brunauer–Emmett–Teller, Ref. 11)
  - BET constant K_B (dimensionless), the monolayer adsorption capacity c_0 (SI unit: mol/kg) and the saturation concentration, c_S (SI unit: mol/m^3).

These predefined expressions are adsorption isotherms that describe the amount of species sorbed to the solid. Applying the isotherms, as defined in the Adsorption section above, assumes that adsorption is at equilibrium locally. This implies that the species phase transfer, between the fluid and the solid phase (within the porous medium), is much faster than the transport within the fluid phase.

Using a Species Source feature, arbitrary expressions can be entered to define, for example, nonequilibrium and temperature-dependent adsorption laws, in the manner of Fetter (Ref. 12), or Bear and Verruijt (Ref. 13).

The retardation factor, RF, describes how adsorption slows the solute velocity, $\mathbf{u}_c$, relative to the average linear velocity of the fluid, $\mathbf{u}_a$, as in

$$\mathrm{RF} = 1 + \frac{\rho_b}{\theta}\frac{\partial c_P}{\partial c} = \frac{\mathbf{u}_a}{\mathbf{u}_c}$$

If the contaminant moves at the average linear velocity of the fluid for $\mathrm{RF} = 1$. For $\mathrm{RF} > 1$, the contaminant velocity is lower than the fluid velocity owing to residence time on solids.

Reactions

Chemical reactions of all types influence species transport in porous media. Examples include biodegradation, radioactive decay, transformation to tracked products, temperature- and pressure-dependent functions, exothermic reactions, and endothermic reactions. The reactions represent change in species concentration per unit volume porous medium per time. Reaction terms are used on the right-hand side of the governing equation to represent these processes. For reactions in a fluid phase, multiply the expression by the fluid volume fraction θ. Similarly, solid phase reaction expressions include the bulk density, ρ_b, and gas phase reactions include the gas volume fraction, a_v.

The following expressions define some common types of reactions:

$R_{Li} = -\theta\frac{\ln 2}{\lambda_{Li}}c_i$	Radioactive decay — liquid
$R_{Pi} = -\rho_b\frac{\ln 2}{\lambda_{Pi}}\left(\frac{\partial c_{Pi}}{\partial c_i}\right)c_i$	Radioactive decay — solid
$R_{Gi} = -\frac{\ln 2}{\lambda_{Gi}}a_v\left(\frac{\partial c_{Gi}}{\partial c}\right)c_i$	Radioactive decay — gas
$R_{Lk} = \theta\zeta_{Li}c_i$	Creation from parent c_{Li} — liquid
$R_{Pk} = \rho_b\zeta_{Pi}\left(\frac{\partial c_{Pi}}{\partial c_i}\right)c_i$	Creation from sorbed parent c_{Pi} — solid
$R_{Gk} = -\zeta a_v\left(\frac{\partial c_{Gi}}{\partial c}\right)c_i$	Reaction — gas

where λ is the chemical half life, ζ is a reaction rate, and the subscripts L, P, and G denote liquid, solid, and gas phases, respectively. In the equations, the reactions either depend on liquid concentration c_i or solid phase concentrations c_{Pi} obtained using the sorption derivative with c_i or gas phase concentration c_{Gi} depending on the gas volume fraction, the volatilization, and the liquid concentration.

Reaction rates can vary with results from other equations in your model, such as temperature. For example, enter the Arrhenius rate law given in Ref. 14:

$$\zeta_T = \zeta_R \exp\left[\frac{E_a(T - T_R)}{R_u T T_R}\right] \tag{8-38}$$

In Equation 8-38, T denotes the current absolute temperature, T_R denotes the reference absolute temperature, E_a is the activation energy, and R_u is the universal gas constant.

Mass Transport in Fractures

When thin fractures occur in porous media, fluid flow tends to move faster along the fracture than in the surrounding media. The transport of chemical species therefore also occur also faster in the direction of the fractures.

The fluid flow in a fracture can be modeled using Darcy's law formulated in a thin sheet of porous medium (a fracture):

$$\mathbf{u} = \frac{\kappa}{\mu}\nabla_t p$$

Here $\mathbf{u}$ is the tangential Darcy velocity, κ is the fracture permeability, μ the fluid's dynamic viscosity, and $\nabla_t p$ is the tangential gradient of the fluid pressure.

The equation to solve for mass transport of species c_i in a thin fracture, embedded in a porous media, is derived from Equation 8-31. The resulting equation is:

$$d_{\mathrm{fr}}\left(\frac{\partial \rho_b c_{\mathrm{P},i}}{\partial t} + \frac{\partial \varepsilon_p c_i}{\partial t} + \nabla_t \cdot (D_{\mathrm{e},i}\nabla_t c_i) + \mathbf{u}\cdot\nabla_t c_i\right) = d_{\mathrm{fr}} R_i + d_{\mathrm{fr}} S_i + n_0 \tag{8-39}$$

Here d_{fr} is the fracture thickness, $c_{\mathrm{P},i}$ the amount of species adsorbed to (or desorbed from) the porous matrix (moles per unit dry weight of the solid), ε_p is the fracture porosity, and D_e is the effective diffusivity. The first two terms on the right hand side represent source terms from reactions, and n_0 corresponds to out-of plane flux from the adjacent porous domain.

In order to arrive at the tangential differential equation, the gradient is split into the contributions normal and tangential to the fracture:

$$\nabla c_i = \nabla_n c_i + \nabla_t c_i$$

The normal gradient is defined in the direction normal to the boundary representing the fracture and the tangential gradient is defined along the boundary. Assuming that the variations in the normal (thin) direction of the fracture are negligible compared to those in the tangential direction, the gradient is simplified as:

$$\nabla c_i = \nabla_t c_i$$

Using The Transport of Diluted Species in Fractures Interface, the transport along fracture boundaries alone is solved for. In this case the transport in the surrounding porous media neglected and the out-of plane flux n_0 vanishes.

See Fracture for more information about the boundary feature solving Equation 8-39. See for more information about the physics interface solving the equation on boundaries only.

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About Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The **Transport of Diluted Species** interface and the **Transport of Concentrated Species** interface support the inclusion of turbulent mixing via the gradient-diffusion hypothesis which adds the following contribution to the diffusion coefficient tensor:

$$\frac{\nu_T}{Sc_T}\mathbf{I} \tag{8-40}$$

where ν_T is the turbulent kinematic viscosity, Sc_T is the turbulent Schmidt number and $\mathbf{I}$ is the unit matrix. While having the form of a diffusive contribution, Equation 8-40

really models a convective phenomenon and it can therefore only be applied along with convection.

The Schmidt number is typically given a value between 0.7 and 0.72, but it can range between 0.3 and 1.3 (at least) depending on the application.

Theory for the Transport of Concentrated Species Interface

The Transport of Concentrated Species Interface theory is described in this section:

- Multicomponent Mass Transport
- Multicomponent Diffusion: Mixture-Averaged Approximation
- Multispecies Diffusion: Fick's Law Approximation
- Multicomponent Thermal Diffusion
- Turbulent Mixing
- Regularization of Reaction Rate Expression
- References for the Transport of Concentrated Species Interface

Multicomponent Mass Transport

Suppose a reacting flow consists of a mixture with $i = 1, \ldots, Q$ species and $j = 1, \ldots, N$ reactions. Equation 8-2 then describes the mass transport for an individual species:

$$\frac{\partial}{\partial t}(\rho\omega_i) + \nabla \cdot (\rho\omega_i \mathbf{u}) = -\nabla \cdot \mathbf{j}_i + R_i \tag{8-41}$$

where, ρ (SI unit: kg/m^3) denotes the mixture density and $\mathbf{u}$ (SI unit: m/s) the mass averaged velocity of the mixture. The remaining variables are specific for each of the species, i, being described by the mass transfer equation:

- ω_i is the mass fraction (1)
- $\mathbf{j}_i$ (SI unit: kg/(m^2·s)) is the mass flux relative to the mass averaged velocity, and
- R_i (SI unit: kg/ (m^3·s)) is the rate expression describing its production or consumption.

The relative mass flux vector $\mathbf{j}_i$ can include contributions due to molecular diffusion and thermal diffusion.

Summation of the transport equations over all present species gives Equation 8-42 for the conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{8-42}$$

assuming that

$$\sum_{i=1}^{Q} \omega_i = 1, \quad \sum_{i=1}^{Q} \mathbf{j}_i = 0, \quad \sum_{i=1}^{Q} R_i = 0$$

Using the mass conservation equation, the species transport for an individual species, i, is given by:

$$\rho \frac{\partial}{\partial t}(\omega_i) + \rho(\mathbf{u} \cdot \nabla)\omega_i = -\nabla \cdot \mathbf{j}_i + R_i \tag{8-43}$$

$Q - 1$ of the species equations are independent and possible to solve for using Equation 8-43. To compute the mass fraction of the remaining species, COMSOL Multiphysics uses the fact that the sum of the mass fractions is equal to 1:

$$\omega_1 = 1 - \sum_{i=2}^{Q} \omega_i \tag{8-44}$$

Multicomponent Diffusion: Mixture-Averaged Approximation

The mixture-averaged diffusion model assumes that the relative mass flux due to molecular diffusion is governed by a Fick's law type approximation.

Assuming that the diffusive flux, relative to the mass averaged velocity, is proportional to the mole fraction gradient, the mass flux is defined as

$$\mathbf{j}_{\mathrm{md},\,i} = -\rho_i D_i^m \frac{\nabla x_i}{x_i} \tag{8-45}$$

Here ρ_i is the density, and x_i the mole fraction of species i. Using the definition of the species density and mole fraction

$$\rho_i = \rho \omega_i, \; x_i = \frac{\omega_i}{M_i} M$$

Equation 8-45 can be expressed in terms of the mass fractions (ω_i) in the manner of

$$\mathbf{j}_{\mathrm{md},\,i} = -\left(\rho D_i^m \nabla \omega_i + \rho \omega_i D_i^m \frac{\nabla M}{M}\right)$$

Using Equation 8-45 together with the Maxwell–Stefan equations, where isobaric and isothermal conditions have been assumed, the following expression for the mixture-averaged diffusion coefficients can be derived (Ref. 3):

$$D_i^m = \frac{1 - \omega_i}{\sum_{k \neq i}^{N} \frac{x_k}{D_{ik}}} \tag{8-46}$$

If instead the diffusive flux (relative to the mass averaged velocity) is assumed proportional to the mass fraction gradient, the mass flux is defined as

$$\mathbf{j}_{\mathrm{md},\,i} = -\rho_i D_i^{m*} \frac{\nabla \omega_i}{\omega_i} = -\rho D_i^{m*} \nabla \omega_i \tag{8-47}$$

For this assumption, using Equation 8-47 together with the Maxwell–Stefan equations, also assuming isobaric and isothermal conditions, the following expression for the mixture-averaged diffusion coefficients can be derived (Ref. 3):

$$\frac{1}{D_i^{m*}} = \sum_{k \neq i}^{N} \frac{x_k}{D_{ik}} + \frac{x_i}{1 - \omega_i} \sum_{k \neq i}^{N} \frac{\omega_k}{D_{ik}} \tag{8-48}$$

THE MIXTURE-AVERAGED DIFFUSION COEFFICIENT

When using the mixture-averaged model, the diffusion is proportional to a single diffusion coefficient. The coefficient describes the diffusion of species i relative to the remaining mixture and is referred to as the mixture-averaged diffusion coefficient. The coefficient is explicitly given in terms of the multicomponent Maxwell–Stefan diffusivities D_{ik}. For low-density gas mixtures, the D_{ik} components can be replaced by the binary diffusivities for the species pairs present.

MIXTURE DIFFUSION CORRECTION

It should be noted that models for the multicomponent diffusivities based on Fick's law are approximations. One drawback of this is that the net diffusive mass flux, the sum of all mass fluxes relative to the mass averaged velocity, is not constrained to zero. To account for this we add a flux, defined by a correction velocity $\mathbf{u}_c$, to enforce a zero net diffusive flux in the manner of:

$$\sum_{i=1}^{N} \mathbf{j}_{\mathrm{md},i} = \sum_{i=1}^{N} \rho\omega_i(\mathbf{u}_{\mathrm{d},i} + \mathbf{u}_{\mathrm{c}}) = 0 \tag{8-49}$$

Hence the correction velocity is:

$$\mathbf{u}_{\mathrm{c}} = -\sum_{i=1}^{N} \omega_i \mathbf{u}_{\mathrm{d},i} \tag{8-50}$$

Here $\mathbf{u}_{\mathrm{d},i}$ is the diffusion velocity resulting from the flux assumption in Equation 8-45 or Equation 8-47. Note that the correction velocity is a constant correction (same for all species), but varies in space.

Using the correction velocity together with Equation 8-45 (flux proportional to the mole fraction gradient), the resulting diffusive flux is

$$\mathbf{j}_{\mathrm{md},i} = -\rho D_i^m \nabla\omega_i - \rho\omega_i D_i^m \frac{\nabla M}{M} + \rho\omega_i \sum_{i=1}^{N} \frac{M_i}{M} D_i^m \nabla x_i \tag{8-51}$$

If instead Equation 8-47 is used (flux proportional to the mass fraction gradient), the resulting diffusive flux is

$$\mathbf{j}_{\mathrm{md},i} = -\rho D_i^{m*} \nabla\omega_i + \rho\omega_i \sum_{i=1}^{N} D_i^{m*} \nabla\omega_i \tag{8-52}$$

ADDITIONAL TRANSPORT MECHANISMS

Apart from molecular diffusion, transport due to thermal diffusion can be accounted for by adding the following term to the diffusive flux:

$$\mathbf{j}_i = \nabla \cdot \left(D_i^T \frac{\nabla T}{T} \right)$$

Here D_i^T (SI unit: kg/(m·s)) is the thermal diffusion coefficient.

Multispecies Diffusion: Fick's Law Approximation

Using a *Fick's law approximation*, the relative mass flux due to molecular diffusion is governed by

$$\mathbf{j}_{\mathrm{md},i} = -\rho_i D_{i,kl}^F \frac{\nabla x_i}{x_i} \tag{8-53}$$

when assuming that the diffusive flux is proportional to the mole fraction gradient. If instead assuming that it is proportional to the mass fraction it becomes

$$\mathbf{j}_{\mathrm{md},i} = -\rho D^F_{i,kl}\nabla\omega_i \tag{8-54}$$

In the equations above $D^F_{i,kl}$ represents a general diffusion matrix (SI unit: m^2/s) describing the diffusion of species i into the mixture. This form makes it possible to use any diffusion coefficient, matrix, or empirical model based on Fick's law. For example, in situations when the mass transport is not dominated by diffusion, an alternative is to use the diffusion coefficients at infinite dilution,

$$D^F_{i,kk} = D^0_i$$

These coefficients are typically more readily available compared to the binary diffusion diffusivities, especially for liquid mixtures.

The mixture diffusion correction described above for the mixture-averaged diffusion can also be applied in this case. Correspondingly, the resulting diffusive flux is

$$\mathbf{j}_{\mathrm{md},i} = -\rho D^F_{i,kl}\nabla\omega_i - \rho\omega_i D^F_{i,kl}\frac{\nabla M}{M} + \rho\omega_i\sum_{i=1}^{N}\frac{M_i}{M}D^F_{i,kl}\nabla x_i \tag{8-55}$$

when using Equation 8-53 and

$$\mathbf{j}_{\mathrm{md},i} = -\rho D^F_{i,kl}\nabla\omega_i + \rho\omega_i\sum_{i=1}^{N}D^F_{i,kl}\nabla\omega_i \tag{8-56}$$

when instead using Equation 8-54.

When using the Fick's Law approximation, Additional Transport Mechanisms can be accounted for in the same manner as described above for the mixture-averaged approximation.

Multicomponent Thermal Diffusion

Mass diffusion in multicomponent mixtures due to temperature gradients is referred to as the *Soret effect*. This occurs in mixtures with high temperature gradients and large variations in molecular weight (or size) of the species. Typically species with high molecular weight accumulate in lower temperature regions while the diffusion due to the Soret effect transports species with low molecular weight to higher temperature regions. In COMSOL Multiphysics, thermal diffusion is included by prescribing the thermal diffusion coefficients D^T_i. In a multicomponent mixture, the sum of the thermal diffusion coefficients is zero:

$$\sum_{i=1}^{Q} D_i^T = 0$$

Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The Transport of Concentrated Species Interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis. In the case of mixture-averaged diffusion, it adds the following contribution to the diffusion coefficient for each species:

$$\frac{\nu_T}{Sc_T} \tag{8-57}$$

while for Fick's law diffusion, it adds the following contribution to the diffusion coefficient tensor:

$$\frac{\nu_T}{Sc_T}\mathbf{I} \tag{8-58}$$

Here, ν_T is the turbulent kinematic viscosity, Sc_T is the turbulent Schmidt number and $\mathbf{I}$ is the unit matrix. While having the form of diffusive contributions, Equation 8-57 and Equation 8-58 really model a convective phenomenon and they can therefore only be applied along with convection.

The Schmidt number is typically given a value between 0.7 and 0.72, but it can range between 0.3 and 1.3 (at least) depending on the application.

Regularization of Reaction Rate Expression

The flexibility of COMSOL means that a reaction can result in nearly any reaction rate contribution R_i^c to a mass fraction ω_i. But a reactant, ω_r, can physically only be consumed if $\omega_r > 0$ and a product, ω_k, can only be formed if $\omega_k < 1$. The Reaction feature in Transport of Concentrated Species Interface contains a way to regularize make the rate expression contributions comply to these restrictions.

When selected the "core", or unregularized reaction rate contribution, R_i^c, to a mass fraction ω_i is replaced by

$$R_i = \frac{1}{2}\frac{R_i^c - |R_i^c|}{\max(\omega_i, \omega_i^{dl})}\max(\omega_i, 0) + \frac{1}{2}\frac{R_i^c + |R_i^c|}{\max(1-\omega_i, \omega_i^{dl})}\max(1-\omega_i, 0) \qquad (8\text{-}59)$$

The first term on the right hand side of Equation 8-59 is active if $R_i^c < 0$, that is if ω_i is a reactant. The reaction rate contribution, R_i, is equal to the "core" reaction rate, R_i^c, as long as $\omega_i > \omega_i^{dl}$. As ω_i approaches zero, the regularization damps out negative R_i^c and for $\omega_i < 0$, R_i for reactant ω_i is equal to zero.

The second term on the right hand side of Equation 8-59 is active if $R_i^c > 0$, that is if ω_i is a product. The reaction rate contribution, R_i, is equal to the "core" reaction rate, R_i^c, as long as $\omega_i < 1 - \omega_i^{dl}$. As ω_i approaches one, the regularization damps out positive R_i^c and for $\omega_i > 1$, R_i for product ω_i is equal to zero.

The damping limits, ω_i^{dl}, should be in an order of magnitude that can be considered numerical noise for species i. The damping limits are per default set to $1e^{-6}$, which is appropriate for most applications. It can be advantageous to lower some limits when working with for example catalytic trace species and the limits can sometimes be raised to gain additional robustness.

References for the Transport of Concentrated Species Interface

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Theory for the Reacting Flow Interfaces

The following sections describe theory applicable for the Reacting Flow interfaces:

- Pseudo Time Stepping for Mass Transport
- The Stefan Velocity
- The Chemical Reaction Rate
- Nonisothermal Reacting Flow
- Turbulent Mass Transport Models
- Mass Transport Wall Functions
- Turbulent Reactions
- The Reaction Source Term for Turbulent Flow
- Theory for the Interior Fan Boundary Condition
- References for the Reacting Flow Interfaces

Pseudo Time Stepping for Mass Transport

In order to improve the solution robustness, pseudo time stepping can be used for the Transport of Concentrated Species interface when solving a stationary model. Using pseudo time stepping, a fictitious time derivative term:

$$\rho\frac{\omega_i - \text{nojac}(\omega_i)}{\Delta\tilde{t}}$$

is added to the left-hand side of the mass fraction equations. Here ρ is the fluid mixture density, ω_i is the mass fraction (dimensionless) of species i, and $\Delta\tilde{t}$ is the *pseudo time step*. Since ω_i–`nojac`(ω_i) is always zero, this term does not affect the final solution. It

does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a time step of size $\Delta\tilde{t}$.

For a description of the pseudo time step term for the Navier–Stokes equations and the pseudo time step see Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual.*

The Stefan Velocity

Heterogeneous reactions on fluid-solid surfaces can affect the mass, momentum, and energy balances at the interface separating the fluid and the solid. On the reacting surface, the production or destruction rate, $r_{s,i}$ (SI unit: mol/(m^2·s)), of a fluid phase species is balanced by the total mass flux of the species. The mass balance for species i on a boundary representing a fluid-solid interface is given by

$$\mathbf{n} \cdot (\mathbf{j}_i + \rho\omega_i\mathbf{u}) = r_{s,i}M_i \tag{8-60}$$

Here, $\mathbf{n}$ is the unit normal pointing out of the fluid domain, $\mathbf{u}$ is the mass averaged velocity of the fluid mixture (SI unit: m/s), $\mathbf{j}_i$ denotes the mass flux of species i relative to the mixture (typically due to diffusion), and M_i is the species molar mass (SI unit: kg/mol). Summing the mass balances at the surface, over all species, results in an effective mixture velocity:

$$\mathbf{n} \cdot \rho\mathbf{u}_s = \sum_{i=1}^{N} r_{s,i}M_i \tag{8-61}$$

referred to as the Stefan velocity, here denoted $\mathbf{u}_s$. To reach Equation 8-61 the fact that the sum of all mass fractions is one, and that the sum of all relative diffusive fluxes is zero, was used.

Equation 8-61 implies that surface reactions result in a net flux between the surface and the domain. A net flux in turn corresponds to an effective convective velocity at the domain boundary; the Stefan velocity. It should be noted here that when solving for mass transport inside a fluid domain, an outer boundary of the domain corresponds to a position just outside of the actual physical wall (on the fluid side). The domain boundary does not coincide with the physical wall.

In most reacting flow models, the species mass fractions in the fluid domain are solved for without including the surface concentrations (mol per area) on exterior walls. One reason for this is that the surface reaction rates are often not known. In this case, surface reactions can be modeled either by applying a mass flux or prescribing the mass fraction, or a combination of both, on fluid boundaries adjacent to the reacting surface. The Stefan velocity on a fluid domain boundary is then defined as the net mass flux resulting from the boundary conditions applied:

$$\mathbf{n} \cdot \rho \mathbf{u}_s = \sum_{i=1}^{N} \mathbf{n} \cdot (\mathbf{j}_{0,i} + \rho \omega_{0,i} u) \tag{8-62}$$

Here, the first term contains contributions from boundary conditions prescribing the mass flux, while the second contains contributions from boundary conditions prescribing the mass fractions. Contributions to the Stefan velocity can be added by selecting **Account for Stefan velocity** in the Flux or Mass Fraction features in The Transport of Concentrated Species interface.

The resulting Stefan velocity based on mass transport boundary conditions is computed as

$$\mathbf{n} \cdot \mathbf{u}_s = \frac{\sum_{i=1}^{N} \mathbf{n} \cdot \mathbf{j}_{0,i}}{\rho \left(1 - \sum_{i}^{N} \omega_{i,0} \right)} \tag{8-63}$$

Using a Reacting Flow interface, the Stefan velocity, defined in the manner of Equation 8-63, is automatically computed and applied on boundaries corresponding to walls in the coupled fluid flow interface. The Stefan velocity is prescribed in the wall normal direction on the wall selection.

The Chemical Reaction Rate

For laminar flow, or when the **Turbulent-reaction model** is set to **None** in a Reaction feature (in Transport of Concentrated Species), the default (Automatic) reaction rate used by the Reaction feature is based on the mass action law. Consider a general reaction belonging to a set of j reactions and involving i species:

$$\mathrm{aA} + \mathrm{bB} + \cdots \underset{k_j^r}{\overset{k_j^f}{\rightleftharpoons}} \mathrm{xX} + \mathrm{yY} + \cdots \tag{8-64}$$

For such a reaction set, the reaction rates r_j (SI unit: mol/(m^3·s)), can be described by the mass action law:

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}} - k_j^r \prod_{i \in \text{prod}} c_i^{\nu_{ij}} \tag{8-65}$$

Here, k_j^f and k_j^r denote the forward and reverse rate constants, respectively. The concentration of species i is denoted c_i (SI unit: mol/m^3). The stoichiometric coefficients are denoted ν_{ij}, and are defined to be negative for reactants and positive for products. In practice, a reaction seldom involves more than two species colliding in a reacting step, which means that a kinetic expression is usually of order 2 or less (with respect to the involved concentrations).

In addition to the concentration dependence, the temperature dependence can be included by using the predefined Arrhenius expressions for the rate constants:

$$k = AT^n \exp\left(-\frac{E}{R_g T}\right)$$

Here, A denotes the frequency factor, n the temperature exponent, E the activation energy (SI unit: J/mol) and R_g the gas constant, 8.314 J/(mol·K). The pre-exponential factor, including the frequency factor A and the temperature factor T^n, is given the units $(\mathrm{m}^3/\mathrm{mol})^{\alpha-1}/\mathrm{s}$, where α is the order of the reaction (with respect to the concentrations).

Nonisothermal Reacting Flow

When a Chemistry interface and a Heat Transfer interface are used in the Nonisothermal Reacting Flow multiphysics coupling, the heat equation is modified to account for reactions and diffusion.

In presence of chemical reactions, the enthalpy (SI unit: J/kg) is a function of temperature, pressure and the mixture composition. For a mixture of N components, the mass fractions verify the condition $\omega_1 + \ldots + \omega_N = 1$. Therefore the enthalpy is a function of the temperature, pressure, and only $N - 1$ mass fractions:

$$\hat{H} = \hat{H}(T, p, \omega_1, \ldots, \omega_{N-1})$$

Assuming the same velocity for the convection term of all components, the mass fractions follow the equation:

$$\rho\left(\frac{\partial}{\partial t}(\omega_i) + (\mathbf{u}\cdot\nabla)\omega_i\right) = -\nabla\cdot\mathbf{j}_i + R_i$$

On the other hand, using the chain rule, the enthalpy variation is written:

$$\rho\frac{D\hat{H}}{Dt} = \rho\left.\frac{\partial\hat{H}}{\partial T}\right|_{p,\,\omega_j}\frac{DT}{Dt} + \rho\left.\frac{\partial\hat{H}}{\partial p}\right|_{T,\,\omega_j}\frac{Dp}{Dt} + \rho\sum_{i=1}^{N-1}\left.\frac{\partial\hat{H}}{\partial\omega_i}\right|_{T,\,p,\,\omega_{j\neq i}}\frac{D\omega_i}{Dt}$$

which can be rewritten using the partial molar enthalpies:

$$\overline{H}_i = \left.\frac{\partial\hat{H}}{\partial n_i}\right|_{T,\,p,\,n_{j\neq i}}$$

$$\rho\frac{D\hat{H}}{Dt} = \rho\left.\frac{\partial\hat{H}}{\partial T}\right|_{p,\,\omega_j}\frac{DT}{Dt} + \rho\left.\frac{\partial\hat{H}}{\partial p}\right|_{T,\,\omega_j}\frac{Dp}{Dt} + \sum_{i=1}^{N}\frac{\overline{H}_i}{M_i}(-\nabla\mathbf{j}_i + R_i)$$

Additionally, the heat balance equation in terms of internal energy is written:

$$\rho\frac{DE}{Dt} = -\nabla\cdot\mathbf{q} + Q_{\mathrm{vd}} + Q$$

where Q_{vd} is the heat source from viscous dissipation, and Q represents additional sources. The heat flux $\mathbf{q}$ consists in a term of conduction and a term of diffusion:

$$\mathbf{q} = \mathbf{q}_{\mathrm{cond}} + \mathbf{q}_{\mathrm{diff}} = -k\nabla T + \sum_{i=1}^{N}\frac{\overline{H}_i}{M_i}\mathbf{j}_i$$

Enthalpy and internal energy are linked through the formula $E = \hat{H} - \frac{p}{\rho}$, we can thus rewrite the heat balance equation in terms of enthalpy:

$$\rho\left.\frac{\partial\hat{H}}{\partial T}\right|_{p,\,\omega_j}\frac{DT}{Dt} + \left(\rho\left.\frac{\partial\hat{H}}{\partial p}\right|_{T,\,\omega_j} - 1\right)\frac{Dp}{Dt} + \sum_{i=1}^{N}\frac{\overline{H}_i}{M_i}(-\nabla\mathbf{j}_i + R_i) = -\nabla\cdot\mathbf{q} + Q_{\mathrm{vd}} + Q$$

Introducing the heat capacity at constant pressure C_p (SI unit: J/(kg·m^3), and the coefficient of thermal expansion α_p (SI unit: 1/K) gives:

$$\rho C_p \frac{DT}{Dt} - \alpha_p T \frac{Dp}{Dt} + \sum_{i=1}^{N} \frac{\overline{H}_i}{M_i}(-\nabla \mathbf{j}_i + R_i) = -\nabla \cdot \mathbf{q} + Q_{\mathrm{vd}} + Q$$

The term with the pressure derivative is the work of pressure forces Q_p. The enthalpy variation due to the gradient of species mass flux can be partly simplified with the diffusion part of the heat flux. The heat source of reaction can be written in terms of enthalpies of reaction H_i instead of partial enthalpies (see Ref. 9). The temperature derivative term can be expanded to make the convective term appear. We finally obtain the temperature equation for a free flow with N species and M reactions:

$$\rho C_p \left[\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T\right] + \nabla \cdot (-k\nabla T) = Q_{\mathrm{diff}} + Q_{\mathrm{react}} + Q_{\mathrm{vd}} + Q_p + Q$$

$$Q_{\mathrm{diff}} = -\sum_{i=1}^{N} \mathbf{j}_i \cdot \nabla\left(\frac{\overline{H}_i}{M_i}\right)$$

$$Q_{\mathrm{react}} = -\sum_{i=1}^{M} H_i r_i$$

$$Q_{\mathrm{vd}} = (-p\mathbf{I} + \tau) : \nabla \mathbf{u}$$

$$Q_p = \alpha_p T \left[\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p\right]$$

For reacting flows moving through the interstices of a porous medium, the heat sources of reaction and diffusion are only accounted for the temperature of the fluid phase. While the porosity is already accounted for in the diffusion term through the mass flux, the heat source of reaction has to be multiplied by the porosity. Also, in presence of a porous catalyst, both reactions in the bulk and reactions at the surface are accounted for in the reaction source term:

$$Q_{\mathrm{react}} = -\varepsilon_{\mathrm{p}} \sum_{i=1}^{M_{\mathrm{bulk}}} H_i r_i - S_{\mathrm{area}} \sum_{i=1}^{M_{\mathrm{surf}}} H_i^{\mathrm{s}} r_i^{\mathrm{s}}$$

where ε_p is the porosity of the medium (SI unit: 1), S_{area} is the specific surface area (SI unit: 1/m), and r_i^{s} is the surface reaction rate (SI unit: mol/(m^2·s)).

An additional source term is added to model convective heat transfer between the fluid and the porous matrix to get the temperature equation for nonisothermal reacting flows in porous media:

$$\rho_f C_{p,f}\left[\frac{\partial T_f}{\partial t} + (\mathbf{u}\cdot\nabla)T_f\right] + \nabla\cdot(-k_f\nabla T_f) = Q_{diff} + Q_{react} + Q_{vd} + Q_p + Q_{s,f} + Q$$

This equation is the one that is solved when the **Porous medium type** of the Porous Medium feature is set to **Local thermal nonequilibrium**, since both fluid and porous matrix temperatures are solved separately. With the **Local thermal equilibrium** approach, the equation is written for the common temperature, and in terms of effective material properties for the time derivative term and conduction term:

$$(\rho C_p)_{eff}\frac{\partial T}{\partial t} + \rho_f C_{p,f}(\mathbf{u}\cdot\nabla)T + \nabla\cdot(-k_{eff}\nabla T) = Q_{diff} + Q_{react} + Q_{vd} + Q_p + Q$$

Turbulent Mass Transport Models

The RANS turbulence models included in the Reacting Flow interfaces are based on averaging of the fluid flow equations. Applying a corresponding decomposition of the fluctuating mass fraction, into mean and fluctuating parts, and averaging the mass transport equations, additional unclosed terms are introduced in the equations. These terms need to be modeled in order to close the set of equations. The most important terms, containing the correlations of the velocity and mass fraction fluctuations, referred to as the turbulent mass transport fluxes, are given by

$$\frac{\partial(\overline{\rho u_i'' \omega''})}{\partial x_i}$$

Here the double primes denote Favre (density-based) fluctuations. In the case of varying density flow, Favre averaging is favored over Reynolds averaging since it reduces the number of unclosed terms and renders the equation on the same form as the incompressible RANS equations. For more background on averaging, see Turbulence Modeling.

The most common way to model this term is to use a gradient based assumption, where the additional turbulent transport is related to the turbulent viscosity through a turbulent Schmidt number Sc_T:

$$\overline{\rho u_i'' \omega''} = -\frac{\mu_T}{Sc_T}\frac{\partial \tilde{\omega}}{\partial x_i} = -\rho D_T \frac{\partial \tilde{\omega}}{\partial x_i} \tag{8-66}$$

Here $\tilde{\omega}$ denotes the Favre-averaged mass fraction which is the quantity solved for.

Using a RANS turbulence model, the turbulent mass flux is defined from Equation 8-66, and the equation solved for each species is

$$\bar{\rho}\frac{\partial}{\partial t}(\tilde{\omega}_i) + \bar{\rho}(\tilde{\mathbf{u}} \cdot \nabla)\tilde{\omega}_i =$$
$$\nabla \cdot \left(\bar{\rho}\left(D_i + \frac{\nu_T}{Sc_T}\right)\nabla\tilde{\omega}_i + \bar{\rho}\tilde{\omega}_i D_i \frac{\nabla M}{M} + \bar{D}_i^T \frac{\nabla T}{T} + \bar{\rho}\tilde{\omega}_i z_i u_{m,i} F \nabla V\right) + R_i$$

where the molecular diffusion coefficient, D_i, is given by the diffusion model (Mixture-Average or Fick's Law).

When modeling transport of dilute solutes in a solvent, for example using the Transport of Diluted Species interface, the species concentration are solved for and the most important unclosed turbulent transport terms correspond to

$$\frac{\partial(\overline{u_i' c'})}{\partial x_i}$$

Here primes indicate turbulent fluctuations from a Reynolds averaging. Using a gradient-based assumption, the additional turbulent transport is modeled as

$$\overline{u_i' c'} = -\frac{\eta_T}{Sc_T}\frac{\partial c}{\partial x_i} = -D_T \frac{\partial c}{\partial x_i} \tag{8-67}$$

where c represents the average concentration. Using a RANS turbulence model the equations solved for the concentration of each species is

$$\frac{\partial c}{\partial t} + (\mathbf{u} \cdot \nabla)c_i =$$
$$\nabla \cdot \left(\left(D_i + \frac{\nu_T}{Sc_T}\right)\nabla c_i + c_i z_i u_{m,i} F \nabla V\right) + R_i \tag{8-68}$$

KAYS–CRAWFORD

Assuming that the turbulent transport mechanisms of heat and mass processes are analogous, the turbulent Schmidt number is defined by (Ref. 1)

$$Sc_T = \left(\frac{1}{2Sc_{T\infty}} + \frac{0.3Pe_T}{\sqrt{Sc_{T\infty}}} - (0.3Pe_T)^2[1 - e^{-1/(0.3Pe_T\sqrt{Sc_{T\infty}})}]\right)^{-1}$$

where the Schmidt number at infinity is $Sc_{T\infty} = 0.85$, and the turbulent Peclet number is defined as the ratio of the turbulent to molecular viscosity times the Schmidt number:

$$Pe_T = \frac{\nu_T}{\nu} Sc$$

HIGH SCHMIDT NUMBER MODEL

In the case of high Schmidt numbers, which is typical for mass transport in liquids, the mass transfer near walls can be significantly different than that for Schmidt numbers of order unity. A diffusion layer near a solid wall, due to, for example, a reaction on the wall, does not have the same properties as the (momentum) boundary layer. Most importantly the diffusion layer thickness is significantly smaller than the boundary layer thickness for high Schmidt numbers. To correctly capture the mass flux at the wall, the wall resolution required is dictated by the diffusion layer rather than by the boundary layer.

The High Schmidt number model is based on the model by Kubacki and Dick (Ref. 2) and is available when using the Low-Reynolds k-ε turbulence model, the SST turbulence model, or the k-ω turbulence model together with Low Re wall treatment. In this case the fluid flow is resolved all the way to the physical wall and consequently, and species boundary equations are applied directly on the wall (without using wall functions).

In the near wall region, where the species transport is limited by diffusion, the mass diffusivity is modeled using an analytical function of the nondimensional wall distance due to Na and Hanratty (Ref. 3):

$$\frac{D_{T,w}}{\nu} = b(l^*)^m$$

The nondimensional wall distance applied, l^*, corresponds to that defined by the turbulence model. The value of the constants b and m are given in Table 8-1.

TABLE 8-1: NA AND HANRATTY PARAMETERS.

SCHMIDT NUMBER	b	m
0.1 < Sc < 5	$7.3 \cdot 10^{-4}$	3
5 < Sc < 50	$5.3 \cdot 10^{-4}$	3
Sc > 50	$4.63 \cdot 10^{-4}$	3.38

Further out from the wall, where the mass transport is governed by the turbulent transport, the transport is modeled using a turbulent Schmidt number of the form (Ref. 2)

$$\mathrm{Sc}_{\mathrm{T,c}} = \left(0.5882 + 0.228\left(\frac{\nu_\mathrm{T}}{\nu}\right) - 0.0441\left(\frac{\nu_\mathrm{T}}{\nu}\right)^2 \left[1 - e^{-5.165/(\nu_\mathrm{T}/\nu)}\right]\right)^{-1}$$

In order to combine the two descriptions, the blending function by Kader (Ref. 4) is used:

$$D_\mathrm{T} = \frac{\nu_\mathrm{T}}{\mathrm{Sc}_{\mathrm{T,c}}} e^{(-\Gamma)} + D_{\mathrm{T,w}} e^{(-1/\Gamma)}$$

where

$$\Gamma = \frac{0.01(l^*)^4}{(1 + 5l^*)}$$

Mass Transport Wall Functions

Analogous to the single-phase flow wall functions (see Wall Functions applied for the Wall boundary condition), there is a theoretical gap between the solid wall and the computational domain of the fluid. This gap is often ignored when the computational geometry is drawn.

Assuming that the turbulent heat and mass transfer in the near-wall region are analogous, the same type of wall functions used for the temperature (Ref. 8) is also applicable for the mass transport. The mass transfer wall function is formulated as a function of the molecular and turbulent Schmidt numbers of each species, instead of the corresponding Prandtl numbers.

Assume that there is a mass fraction $\omega_{i,\mathrm{w}}$ just outside the wall and that it is in equilibrium with the surface chemistry. The mass flux, for species i, between the wall and a fluid with a mass fraction of $\omega_{i,\mathrm{f}}$ at the lift-off position is

$$m_\mathrm{wf} = \frac{\rho C_\mu^{1/4} k^{1/2} (\omega_{i,\,\mathrm{w}} - \omega_{i,\,\mathrm{f}})}{\omega_i^+}$$

where ρ is the fluid density, C_μ is a turbulence modeling constant, and k is the turbulent kinetic energy. ω_i^+ is the dimensionless mass fraction given by (Ref. 8)

$$\omega_i^+ = \begin{cases} \mathrm{Sc}\delta_w^+ & \text{for } \delta_w^+ < \delta_{w1}^+ \\ \left(15\mathrm{Sc}^{2/3} - \dfrac{500}{\delta_w^{+2}}\right) & \text{for } \delta_{w1}^+ \le \delta_w^+ < \delta_{w2}^+ \\ \dfrac{\mathrm{Sc}_T}{\kappa}\ln\delta_w^+ + \beta & \text{for } \delta_{w2}^+ \le \delta_w^+ \end{cases}$$

where in turn

$$\delta_w^+ = \frac{\delta_w \rho \sqrt{C_\mu^{1/2} k}}{\mu} \qquad \delta_{w1}^+ = \frac{10}{\mathrm{Sc}^{1/3}}$$

$$\delta_{w2}^+ = 10\sqrt{10\frac{\kappa}{\mathrm{Sc}_T}} \qquad \mathrm{Sc} = \frac{\mu}{\rho D_{i,\,m}}$$

$$\beta = 15\mathrm{Sc}^{2/3} - \frac{\mathrm{Sc}_T}{2\kappa_v}\left(1 + \ln\left(1000\frac{\kappa}{\mathrm{Sc}_T}\right)\right)$$

κ_v is the von Kármán constant, and $D_{i,\mathrm{m}}$ the mean species diffusion coefficient. The latter corresponds directly to the mixture-averaged diffusion coefficient when using the Mixture-average diffusion model. Using the Fick's law diffusion model, the mean diffusion coefficient is computed as $1/N \cdot \mathrm{tr}(\boldsymbol{D}_i)$, where $\boldsymbol{D}_i$ is the diffusion tensor and N is the dimension of the model.

The computational result should be checked so that the distance between the computational fluid domain and the wall, δ_w, is almost everywhere small compared to any geometrical quantity of interest. The distance δ_w is available as a postprocessing variable (`delta_w`) on boundaries.

Turbulent Reactions

In turbulent flow the reaction rate is significantly affected by the turbulence. Turbulent fluctuations can increase the reaction rate due to the increased mixing, but it can also quench it through removal of species or the heat required for ignition. The interaction between the flow and the reactions can be quantified through the Damköhler number Da:

$$\mathrm{Da} = \frac{\tau_T}{\tau_c}$$

which compares the time scale of the largest turbulent flow structures (the integral time scale), to the chemical time scale. In the limit of large Damköhler numbers $\mathrm{Da} >> 1$, the reactive time scale is significantly smaller than that of the turbulence. In this regime the inner structure of a reaction zone is thin enough not to be affected by turbulence. The reacting regions are, however, convected and wrinkled by the turbulence. In this case the global reaction rate is proportional to the chemical reaction rate times the surface of the reacting regions. In the limit of small Damköhler numbers $\mathrm{Da} << 1$, the chemical time scale is much larger than that of the turbulent flow. In this case the global reaction rate is controlled by the chemistry, while the turbulence acts by continuously mixing the species. This regime is referred to as a "perfectly stirred reactor".

MEAN VALUE CLOSURE

A mean turbulent production rate can be obtained by directly applying the mean concentrations and temperature in the kinetic reaction rate expressions:

$$R_i = \nu_i M_i r_{\mathrm{MVC},i}$$

where ν_i denotes the species stoichiometric coefficient, M_i the molar mass (SI unit: kg/mol), and $r_{\mathrm{MVC},i}$ is the reaction rate from Equation 8-65 using mean quantities.

This is referred to as mean value closure of the turbulent reaction rate, and corresponds to keeping the first term in a Taylor series expansion of the turbulent reaction rate following a Reynolds decomposition of the fluctuating variables (Ref. 5). The mean value closure is directly applicable in the perfectly-stirred-reactor limit ($\mathrm{Da} << 1$). In this case the turbulence is able to mix the species in the sense of changing the mean concentration, but the turbulent fluctuations do not affect the chemical reaction rate. The mean value closure is also applicable in the limit of low turbulence levels since the turbulent fluctuations tend to zero as the laminar flow regime is approached.

EDDY DISSIPATION MODEL

The eddy-dissipation model for the mean reaction rate originally developed by Magnussen and Hjertager (Ref. 6) for nonpremixed combustion. Using this reaction model, the mean production rate of species i is defined as

$$R_i = \nu_i M_i \frac{\alpha}{\tau_{\mathrm{T}}} \rho \cdot \min\left[\min\left(\frac{\omega_r}{\nu_r M_r}\right), \beta \sum_p \left(\frac{\omega_p}{\nu_p M_p}\right)\right] = \nu_i M_i r_{\mathrm{ED},i}$$

The model assumes that both the Reynolds and Damköhler numbers are sufficiently high for the reaction rate to be limited by the turbulent mixing time-scale τ_T. The reaction can hence at most progress at the rate at which fresh reactants are mixed, at the molecular level, by the turbulence present. Furthermore the reaction rate is limited by the deficient reactant; the reactant with the lowest local concentration. When the model parameter β is finite, the existence of product species is also required for reaction, modeling the activation energy required for reaction (ignition). For gaseous nonpremixed combustion the model parameters have been found to correspond to (Ref. 6)

$$\alpha = 4\,,\ \beta = 0.5$$

For liquid reactions it is recommended that the model parameters are calibrated against experimental or simulation data. Using a mix of the mean value closure and a modified version of the eddy-dissipation model Bakker and Fasano (Ref. 7) found the following parameter values:

$$\alpha_2 = 0.08\,,\ \alpha_1 = \beta_1 = \beta_2 = \infty$$

to give good results for a competitive reaction pair when compared with experimental results.

A common approximation for the turbulence mixing time-scale τ_T is $\tau_T \approx k/\varepsilon$ (Ref. 5). Due to realizability constraints, a more accurate approximation is however

$$\tau_T = \min\left(\frac{k}{\varepsilon}, \frac{1}{C_\mu 3\lambda_{max}}\right) \tag{8-69}$$

where in turn

$$\lambda_{max} = \frac{1}{2}\sqrt{S_{ij}S_{ij}}$$

for 2D and

$$\lambda_{max} = \sqrt{\frac{2S_{ij}S_{ij}}{3}}$$

for 3D and 2D axisymmetry. Equation 8-69 is directly applicable to the k-ε model. For the k-ω and SST turbulence models, Equation 8-69 reads

$$\tau_T = \min\left(\frac{1}{\beta^*\omega}, \frac{1}{\beta^* 3\lambda_{max}}\right)$$

Equation 8-69 is used also for the low-Reynolds k-ε model even though k/ε is not actually the turbulence mixing time scale. To obtain a consistent turbulence mixing time scale for low-Reynolds k-ε, k/ε needs to be multiplied by a damping function that goes to zero at solid walls. Ref. 5 does however notice that τ_T is not a relevant time scale close to walls since it is too small. The damping function is therefore neglected in the eddy-dissipation model.

The Reaction Source Term for Turbulent Flow

For turbulent flow, or when the **Turbulent-reaction model** is set to **Eddy-dissipation** in the Reaction feature (in Transport of Concentrated Species), the reaction source term is computed as the minimum of the mean value closure and that from the eddy dissipation model:

$$R_i = \nu_i M_i \cdot \min\left[r_{\mathrm{MVC},i}, r_{\mathrm{EDC},i}\right]$$

This approach combines the regimes of the separate models. For fast reactions the reaction rate is limited by the turbulent mixing. At the same time, in regions with low turbulence levels, or low kinetic reactions rates, the latter limits the production rate.

Theory for the Interior Fan Boundary Condition

When the Reacting Flow multiphysics coupling feature is active, the mass fraction fields that are discontinuous over the fan. For each species, ω_i, an outlet mass fraction condition is applied:

- If direction is Along normal vector, the outlet mass fraction $\omega_{i,\,\mathrm{avg}}$ is defined by

$$\left(\int_\Gamma \mathrm{up}(\mathbf{u}\cdot\mathbf{n}\rho)dS\right)\omega_{i,\,\mathrm{avg}} = \int_\Gamma \mathrm{down}(\mathbf{u}\cdot\mathbf{n}\rho\omega_i)dS$$

- If the direction is opposite to normal vector, the outlet temperature T_{avg} is defined by

$$\left(\int_\Gamma \mathrm{down}(\mathbf{u}\cdot\mathbf{n}\rho)dS\right)\omega_{i,\,\mathrm{avg}} = \int_\Gamma \mathrm{up}(\mathbf{u}\cdot\mathbf{n}\rho\omega_i)dS$$

This means that there is no diffusion over the interior fan, and no migration either.

References for the Reacting Flow Interfaces

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9

Thin-Film Flow Interfaces

The physics interfaces described in this section are found under the **Thin-Film Flow** branch ( ).

In this chapter

- The Thin-Film Flow Interfaces
- Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow Interfaces

In this section:

- The Thin-Film Flow Interface (3D)
- The Thin-Film Flow, Domain Interface (2D)
- The Thin-Film Flow Interface (2D)
- The Solid–Thin-Film Damping Interface (in the *Structural Mechanics Module User's Guide*)
- Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Interfaces

The physics interfaces found under the **Thin-Film Flow** branch ( ) when adding a physics interface describe momentum transport. These physics interfaces can be added either singularly or in combination with other physics interfaces describing mass and energy transfer. The thin-film flow interfaces are shown in Table 9-1.

TABLE 9-1: THE THIN-FILM FLOW INTERFACES DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	SPACE DIMENSION	GEOMETRIC ENTITY LEVEL
Thin-Film Flow	tff	3D, 2D, 2D axisymmetric	Boundaries
Thin-Film Flow, Domain	tff	2D	Domains

Each of the physics interfaces can be configured to solve either the standard *Reynolds equation* for liquids (with a material or user-defined density specified at the absolute pressure), or the *modified Reynolds equation* for gas flow. The modified Reynolds equation assumes the ideal gas law, and it applies when pressure changes in the flow itself result in significant density changes.

Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow Interface (3D)

The **Thin-Film Flow (tff)** interface ( ), found under the **Thin-Film Flow** branch ( ) when adding a physics interface, is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by a surface within the geometry. It is used for lubrication, elastohydrodynamics, or gas damping simulations

when the fluid channel is thin enough to apply the Reynolds equation or the modified Reynolds equation. The physics interface is available for 3D geometries.

This physics interface is defined on boundaries, which means that the boundary level is the highest level for which this physics interface has equations and features; it does not have any features or equations on the domain level. The boundary represents a reference surface on which the thin-film flow equation is solved. On one side of the boundary level there is a wall and on the other a base surface, neither of which is represented in the geometry. The wall and base surfaces are oriented with respect to the reference surface normal as shown in Figure 9-1. Fluid flows in the gap between the wall and the base.

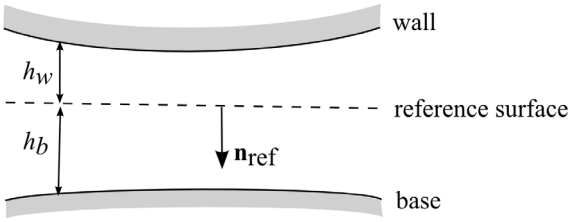


Figure 9-1: Diagram illustrating the orientation of the wall and the base surfaces with respect to the reference surface in the Thin-Film Flow interfaces. A vector from the reference surface to the corresponding point on the wall always points in the $-\mathbf{n}_{\text{ref}}$ direction, where $\mathbf{n}_{\text{ref}}$ is the reference surface normal. Similarly a vector from the reference surface to the corresponding point on the base points in the $+\mathbf{n}_{\text{ref}}$ direction. The height of the wall above the reference surface (h_w) and the height of the base below the reference surface (h_b) are also shown in the figure.

Using equations on the reference surface, the physics interface computes the pressure in a narrow gap between the wall and the base. When modeling the flow, it is assumed that the total gap height, $h = h_w+h_b$, is much smaller than the typical lateral dimension L of the reference surface. The physics interface is used to model laminar flow in thin gaps or channels. A lubricating oil between two rotating cylinders is an example of this.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid-Film Properties**, **Border**, and **Initial Values**. Then, from the **Physics** toolbar, you can add other nodes that implement, for example, boundary conditions. You can also right-click **Thin-Film Flow** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern

<name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is tff.

PHYSICAL MODEL

Select the **Fluid type** — **Liquid (Reynolds equation)**, **Liquid with cavitation**, or **Gas (modified Reynolds equation**).

For **Liquid with cavitation** enter the **Cavitation transition width** (SI unit: Pa). The default is 1 MPa.

Under normal operating conditions, gases dissolved in lubricants cause cavitation when the pressure in the lubricant drops below the saturation pressure. See the theory section for Cavitation for more information.

Some options are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/)

REFERENCE PRESSURE

Enter a **Reference pressure level** p_{ref}. The default value is 1[atm]. This pressure represents the ambient pressure, which is not accounted for when computing fluid loads.

DISCRETIZATION

Select the **Pressure** discretization — **Linear**, **Quadratic**, **Cubic**, or **Quartic** to change the order of the shape functions for the pressure.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure** p_{film}. The name can be changed but the names of fields and dependent variables must be unique within a component.

- Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Interfaces
- Theory for the Thin-Film Flow Interfaces

- *Journal Bearing*: Application Library path **CFD_Module/Thin-Film_Flow/journal_bearing**
- *Tilted Pad Thrust Bearing*: Application Library path **CFD_Module/Thin-Film_Flow/tilted_pad_bearing**

The Thin-Film Flow, Domain Interface (2D)

The **Thin-Film Flow, Domain (tff)** interface ( ), found under the **Thin-Film Flow** branch ( ) when adding a physics interface, is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by a domain within the geometry. It is used for lubrication or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the Modified Reynolds equation to apply. The physics interface is available for 2D geometries.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid-Film Properties**, **Border** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Thin-Film Flow, Domain** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tff`.

The rest of the settings are the same as for The Thin-Film Flow Interface (3D) interface.

- Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Interfaces
- Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow Interface (2D)

The **Thin-Film Flow (tff)** interface ( ) is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by an edge within 2D geometries. It is used for lubrication, elastohydrodynamics, or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the modified Reynolds equation to apply. The physics interface is for 2D and 2D axisymmetric components.

The rest of the settings are the same as for The Thin-Film Flow Interface (3D).

- Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Interfaces
- Theory for the Thin-Film Flow Interfaces

Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Interfaces

For the physics interfaces under the Thin-Film Flow branch, the following domain, boundary, edge, point, and pair nodes (listed in alphabetical order) are described in this section:

- Border
- Fluid-Film Properties
- Initial Values
- Inlet
- Interior Wall
- Mass Source
- Perforations
- Outlet
- Symmetry
- Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid-Film Properties

Use the **Fluid-Film Properties** node to set the wall properties, base properties, fluid properties, and the film flow model.

REFERENCE SURFACE PROPERTIES

In the **Thin-Film Flow (tff)** 2D and 3D interfaces, the **Reference normal orientation** setting allows you to reverse the direction of the reference surface normal used by the physics interface. By default this is set to **Same direction as geometry normal**. To reverse the direction, select **Opposite direction to geometry normal**.

In the **Thin-Film Flow, Domain (tff)** interface, the **Reference surface normal orientation** setting allows you to set the direction of the reference normal so that it either points out of or into the 2D plane. By default this is set to **Reference surface normal points out of plane**, such that the reference surface normal is given by the **z** direction {0,0,1}. Selecting **Reference surface normal points into plane** sets the reference surface normal to {0,0,-1}.

WALL PROPERTIES

Enter a value or expression for the **Height of wall above reference plane** h_{w1} (SI unit: m). The default is 10 µm.

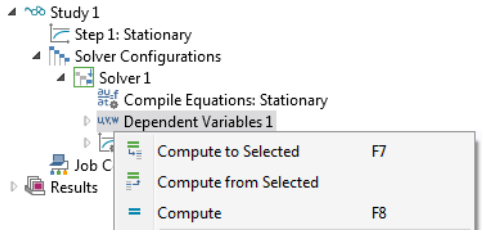
By default the **Additional wall displacement** is **User defined**. Enter values or expressions for $\mathbf{u}_w$ (SI unit: m). The defaults are 0 m. Alternatively select a feature input (defined by a separate physics interface) or **None** from the list.

When using a feature input to define an additional displacement based on the movement of a structure, refer to Figure 9-1 to decide whether the additional displacement should be added to the wall or the base.

- If the reference normal points out of the structure for which the displacement is provided, the structure should be considered to be the wall, and its displacement should be added to the additional wall displacement.

If the reference normal points into the structure for which the displacement is provided, the structure is the base and its displacement should be added to the additional base displacement.To determine the reference normal orientation before fully solving the model, click **Show Default Solver** ( ) in the **Study** toolbar (or right-click the **Study 1** node and select **Show Default Solver**). Then expand the **Study 1**

> **Solver Configurations** > **Solver 1** node, right-click the **Dependent variables** subnode and select **Compute to Selected**.



You can then add a 2D or 3D plot group with an **Arrow Surface** plot (in 3D) ( ) or **Arrow Line** plot (in 2D) ( ), and use the **Replace Expression** ( ) button to plot the **Reference surface normal**.

Note that the orientation of the reference surface normal can be changed using the **Reference normal orientation** setting in the Reference Surface Properties section.

Select a **Wall velocity** $\mathbf{v}_w$ (SI unit: m/s) — **None** (the default), **Calculate from wall displacement**, or **User defined**. For **User defined**, the **Compute implicit height change from wall velocity** checkbox is selected by default. Enter values or expressions for the components of $\mathbf{v}_w$ (SI unit: m/s). The defaults are 0 m/s.

BASE PROPERTIES

See Wall Properties above for details to help you decide whether the additional displacement should be added to the wall or the base.

Enter a value or expression for the **Height of base below reference plane** h_{b1} (SI unit: m). The default is 0 m.

By default **Additional base displacement** is **User defined**. Enter values or expressions for $\mathbf{u}_b$ (SI unit: m). The defaults are 0 m. Or select **None** from the list.

Select a **Base velocity** $\mathbf{v}_b$ (SI unit: m/s) — **None** (the default), **Calculate from base displacement**, or **User defined**. For **User defined**, the **Compute implicit height change from base velocity** checkbox is selected by default. Enter values or expressions for the components of $\mathbf{v}_b$ (SI unit: m/s). The defaults are 0 m/s.

FLUID PROPERTIES

The default **Dynamic viscosity** μ (SI unit: Pa·s) is taken **From material**. For **User defined** enter a different value or expression. The default is 0 Pa·s.

With the default options, the **Density** ρ (SI unit: kg/m^3) is taken **From material**. For **User defined** enter a different value or expression. The default is 0 kg/m^3.

When **Gas (modified Reynolds equation)** is selected in the Physical Model section, the density is determined by the ideal gas law.

When **Liquid with cavitation** is selected in the Physical Model section, the density depends on the pressure as $\rho = \rho_c \exp(\beta p_{\text{film}})$ where p_{film} is the fluid pressure, ρ_c is the density at the cavitation pressure, and β is the fluid compressibility (SI unit: $1/\text{Pa}$). In this case enter the values for the **Density at cavitation pressure** ρ_c (SI unit: Pa) and the **Compressibility** β (SI unit: $1/\text{Pa}$).

FILM FLOW MODEL

Select a **Film flow model** — **No-slip walls** (the default), **Slip at walls**, **User defined-relative flow function**, or **User defined-general**. The film flow model is used to compute the mean fluid velocity as a function of the pressure gradient, the wall velocity, and the base velocity. Within the gap the fluid velocity profile is a linear combination of the Poiseuille and Couette velocity profiles.

No-slip Walls

This flow model assumes no slip at both the wall and base surfaces. Thus the average fluid velocity is computed by assuming that the fluid velocity at the wall and base is equal to the wall and base velocity, respectively.

Slip at Walls

Use **Slip at walls** when slip occurs at the wall and/or the base. In this case the difference between the wall or base velocity and the fluid velocity is proportional to the tangential part of the normal stress tensor component. The slip length divided by the fluid viscosity is the constant of proportionality in this relationship. The mean fluid velocity is computed using this assumption, given the pressure gradient and the wall and base velocities.

Enter a **Slip length, wall** L_{sw}. The default is 0.1 µm.

Select the **Use different slip length for base** checkbox to enter a **Slip length, base** L_{sb}. The default is 0.1 µm.

For **Gas (modified Reynolds equation)** it is possible to use the gas mean free path to specify the slip length. Change the **Type of Slip** setting (which defaults to **Slip Length**

with the settings described above) to **Mean free path and same accommodation coefficients** or to **Mean free path and different accommodation coefficients**.

- For **Mean free path and same accommodation coefficients** enter a value for the **Wall and base accommodation coefficient** α (dimensionless). The default is 0.9.
- For **Mean free path and different accommodation coefficients** enter values for the **Wall accommodation coefficient** α_w (dimensionless, default 0.9) and the **Base accommodation coefficient** α_b (dimensionless, default 0.9).

Define the **Mean free path** — **Compute from material properties** (the default), **User defined expression**, or **User defined with reference pressure**.

- For **User defined expression** enter an expression for the **Mean free path** λ (SI unit: m). The default expression is `((70[nm])*(1[atm]))/(tff.ptot)`.
- For **User defined with reference pressure** enter values for the **Mean free path at reference pressure** λ_0 (SI unit: m; the default is 70 nm), and for the **Mean free path reference pressure** $p_{\lambda 0}$ (SI unit: Pa; the default is 1 atm).

Rarefied-Total Accommodation for Gas (Modified Reynolds Equation)

The **Rarefied-total accommodation** option provides a rarefied gas model that assumes total accommodation at the wall and the base. This model is accurate to within 5% over the range $0 < \mathrm{Kn} < 880$ (here Kn is the Knudsen number, which is the ratio of the mean free path to the film thickness). An empirical function, fitted to stationary solutions of the Boltzmann equation, is used to define the Poiseuille component of the flow.

Define the **Mean free path** — **Compute from material properties** (the default), **User defined expression**, or **User defined with reference pressure**.

- For **User defined expression** enter an expression for the **Mean free path** λ (SI unit: m). The default expression is `((70[nm])*(1[atm]))/(tff.ptot)`.
- For **User defined with reference pressure** enter values for the **Mean free path at reference pressure** λ_0 (the default is 70 nm) and for the **Mean free path reference pressure** $p_{\lambda 0}$ (the default is 1 atm).

Select the **Force model**:

- **Normal-pressure forces only** (the default) to include only the normal pressure forces in the model.

- **Couette (slide film) forces only** to include only the shear forces generated from an empirical model of the rarefied flow developed for pure Couette flows.
- **Shear and normal forces** to include both the shear and pressure forces, combining the other two force models.

Rarefied-General Accommodation for Gas (Modified Reynolds Equation)

The **Rarefied-general accommodation** option provides a rarefied gas model that assumes the same accommodation coefficient, α, at the wall and the base. This model is accurate to within 1% over the ranges $0.7<\alpha<1$ and $0.01<\mathrm{Kn}<88$ (here Kn is the Knudsen number, which is the ratio of the mean free path to the film thickness). An empirical function, fitted to stationary solutions of the Boltzmann equation, is used to define the Poiseuille component of the flow.

Define the **Mean free path** — **Compute from material properties** (the default), **User defined expression**, or **User defined with reference pressure**.

- For **User defined expression** enter an expression for the **Mean free path** λ (SI unit: m). The default expression is `70[nm]*1[atm]/tff.ptot`.
- For **User defined with reference pressure** enter values for the **Mean free path at reference pressure** λ_0 (the default is 70 nm) and for the **Mean free path reference pressure** $p_{\lambda 0}$ (the default is 1 atm).

Select the **Force model**:

- **Normal-pressure forces only** (the default) to include only the normal pressure forces in the model.
- **Couette (slide film) forces only** to include only the shear forces generated from an empirical model of the rarefied flow developed for pure Couette flows.
- **Shear and normal forces** to include both the shear and pressure forces, combining the other two force models.

User Defined-Relative Flow Function

The **User defined-relative flow function** option enables user-defined models in which an effective fluid viscosity is employed. The fluid viscosity is divided by an additional factor Q_{ch}, which can be defined as an arbitrary expression. It is also possible to define the expressions for the fluid forces on the wall and base (these are included as feature inputs in other physics interfaces).

Enter values or expressions for:

- **Relative flow rate function** Q_{ch}. The default is 0 (dimensionless).

- **Fluid load on wall** $\mathbf{f}_w$. The defaults are 0 N/m^2.
- **Fluid load on base** $\mathbf{f}_b$. The defaults are 0 N/m^2.

User Defined — General

The **User defined-general** option allows for arbitrary flow models to be defined. Both the Poiseuille and Couette terms in the mean velocity can be defined arbitrarily. It is also possible to define the expressions for the fluid forces on the wall and base, (these are included as feature inputs in other physics interfaces).

Enter values or expressions for:

- **Poiseuille mean fluid velocity coefficient** $v_{ave,P}$. The default is 0 $m^3 \cdot s/kg$.
- **Couette mean fluid velocity component** $\mathbf{v}_{ave,C}$. The defaults are 0 m/s.
- **Fluid load on wall** $\mathbf{f}_w$. The defaults are 0 N/m^2.
- **Fluid load on base** $\mathbf{f}_b$. The defaults are 0 N/m^2.

Arrow Line and Arrow Surface in the *COMSOL Multiphysics Reference Manual*

Border

Use the **Border** node to set a pressure condition at the border and the border flow type.

The **Border flow** condition is used to account for the pressure drop caused by the flow converging into the gap, outside the thin layer. The acoustic elongation options does this by adding additional thickness to the thin layer beyond the edge of the geometry (assuming a pressure gradient in this layer equal to that at the boundary). The Out-of-plane motion calculates the pressure gradient due to circulation of the fluid caused by motion of the wall or base surfaces using a predefined model. Alternatively the pressure gradient at the boundary can be specified using an arbitrary expression, which allows for more sophisticated, user-defined models.

BORDER SETTINGS

Select a **Border condition** — **Zero pressure** (the default), **Pressure**, or **Border flow**. The option **Starvation** is also available when **Liquid with cavitation** is selected in the Physical Model settings.

- For **Pressure** enter a **Pressure** p_{film0} (SI unit: Pa) to define $p_{\text{film}} = p_{\text{film0}}$ on the boundary, edge, or point. The default is 0 Pa.

  If the reference pressure $p_{\text{ref}} = 0$ in the Reference Pressure section, then p_{film0} represents the absolute pressure; otherwise, p_{film0} sets the relative pressure with respect to p_{ref}.
- For **Border flow** select a **Border flow type** — **Acoustic boundary condition-absolute elongation**, **Acoustic boundary condition-relative elongation**, **Out-of-plane motion**, or **User defined**.
- For **Acoustic Boundary condition-absolute elongation** enter a **Border elongation** ΔL. The default is 0.1 µm.
- For **Acoustic boundary condition-relative elongation** enter a **Relative border elongation** ΔL_r. The default is 0.7 (dimensionless).
- For **Out-of-plane motion** enter the **Model coefficients** η, ζ, χ with defaults 0, 0, 1, respectively. Also enter the **Slip length**, Λ (SI unit: m). The default slip length uses an `if` condition to set the slip length equal to that defined in the Fluid-Film Properties node when a suitable **Film flow model** is selected. If the slip length is not defined in the Fluid-Film Properties node, it defaults to 0.1µm.

  Note that the coefficients can be specified according to the results given in Ref. 9. The following values are recommended:

$$\chi = \frac{1 + 8.834\left(\frac{\Lambda}{h}\right)}{1 + 5.118\left(\frac{\Lambda}{h}\right)}$$

$$\eta = \frac{0.634 + 1.572\left(\frac{\Lambda}{h}\right)}{1 + 0.537\left(\frac{\Lambda}{h}\right)}$$

$$\zeta = \frac{0.445 + 11.20\left(\frac{\Lambda}{h}\right)}{1 + 5.510\left(\frac{\Lambda}{h}\right)}$$

where h is the gap height. The above expressions are valid in the range $0 \le \Lambda/h \le 1$.

- For **User defined** enter a **Normal pressure gradient**. The default is $p_f/(0.1\ \mu\text{m})\ \text{N/m}^3$.
- For **Starvation** enter a value for the **Fluid fraction** θ_0. The default is 0.6 (dimensionless).

Perforations

Use the **Perforations** node for applications in MEMS devices, where the phenomenon of squeeze-film damping is important. A free-hanging thin plate or the substrate often has an array of etch holes that allow the gas in between to escape. The perforations feature acts as a sink for gas that is proportional to both the ambient pressure and to the pressure difference with respect to the ambient on the other side of the perforated surface. The constant of proportionality is known as the admittance, Y, and it can either be defined directly or determined from the model due to Bao (Ref. 16). The ambient pressure is assumed to be the reference pressure p_{ref} specified in the Reference Pressure section.

Note that this feature applies only when the walls do not have tangential movement.

PERFORATIONS

Select a **Perforation admittance** — **User defined** (the default) or **Bao model**.

For **User defined**, enter a value or expression for Y (SI unit: $\text{m}^2\cdot\text{s/kg}$).

For **Bao model**, choose a **Perforation shape** — **Square** (the default) or **Circular**. Then enter the following inputs as applicable:

- **Side length** s_h (SI unit: m).
- **Hole radius** r_h (SI unit: m).
- **Hole length** l_h (SI unit: m).
- **Hole density** n_h (SI unit: $1/\mathrm{m}^2$).

Initial Values

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver. If more than one set of initial values is required, add additional **Initial Values** nodes from the **Physics** toolbar.

INITIAL VALUES

Enter a value or an expression for the initial value of the **Pressure** p_{film} (SI unit: Pa).

Inlet

Use the **Inlet** node to define an edge or point where fluid enters the gap.

INLET SETTINGS

Select an **Inlet condition** — **Zero pressure** (the default), **Pressure**, or **Normal inflow velocity**. The option **Starvation** is also available when **Liquid with cavitation** is selected in the Physical Model section.

- For **Zero pressure** $p_{\mathrm{film}} = 0$ applies on the boundary, edge, or point.
- For **Pressure** enter the **Pressure** p_{film0} (SI unit: Pa) to impose $p_{\mathrm{film}} = p_{\mathrm{film0}}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure $p_{\mathrm{ref}} = 0$ in the Reference Pressure section, then p_{film0} represents the absolute pressure, otherwise p_{film0} sets the relative pressure with respect to p_{ref}.
- For **Normal inflow velocity** enter a **Normal inflow velocity** U_0. The default is 0 m/s.
- For **Starvation** enter a value for the **Fluid fraction** θ_0. The default is 0.6 (dimensionless).

Outlet

The **Outlet** node defines an edge or point where fluid leaves the gap.

OUTLET SETTINGS

Select an **Outlet condition** — **Zero pressure** (the default), **Pressure**, **Normal outflow velocity**, or **Outflow**. The option **Starvation** is also available when **Liquid with cavitation** is selected in the Physical Model section.

- For **Zero pressure**, $p_{\text{film}} = 0$ applies on the boundary, edge, or point.
- For **Pressure**, enter a **Pressure** p_{film0} (SI unit: Pa) to impose $p_{\text{film}} = p_{\text{film0}}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure $p_{\text{ref}} = 0$ in the Reference Pressure section, then p_{film0} represents the absolute pressure, otherwise p_{film0} sets the relative pressure with respect to p_{ref}.
- For **Normal outflow velocity**, enter a **Normal outflow velocity** U_0. The default is 0 m/s.
- For **Outflow**, the fluid is allowed to leave the gap without explicitly imposing a value of pressure or velocity.
- For **Starvation**, enter a value for the **Fluid fraction** θ_0. The default is 0.6 (dimensionless).

Wall

The **Wall** node prevents fluid flow in the direction perpendicular to the boundary.

Interior Wall

The **Interior Wall** feature is similar to the Wall feature but it applies to both sides of an interior boundary. It allows for discontinuities in the pressure, and can be used to avoid meshing thin structures.

Symmetry

The **Symmetry** node sets the perpendicular component of the average velocity in the gap to zero.

Mass Source

The **Mass Source** node adds a user-defined, general mass source term to the thin-film flow equation. The unit is $\text{kg/m}^2\cdot\text{s}$ for the Reynolds equation and W/m^2 for the modified Reynolds equation.

Theory for the Thin-Film Flow Interfaces

The theory for the different versions of the Thin-Film Flow interfaces are described in this section:

- Thin-Film Flow
- The Reynolds Equation
- Flow Models
- The Modified Reynolds Equation — Gas Flow
- Flow Models for Rarefied Gases
- Frequency-Domain Formulation
- Boundary Conditions
- Cavitation
- References for the Thin-Film Flow Interfaces

Thin-Film Flow

Figure 9-2 shows a typical configuration for the flow in a thin layer. The upper boundary is referred to as the wall, and the lower boundary is referred to as the base. Damping and lubrication forces operate on both surfaces.

In many cases the gap is sufficiently small for the flow to be isothermal. The gap thickness, h, is assumed to be much smaller than the lateral dimensions of the geometry, L. If this is the case, it is possible to neglect inertial effects in the fluid in comparison to viscous effects (for MEMS devices this assumption is reasonable below MHz frequencies). Additionally, the curvature of the reference surface can be ignored when $h/L << 1$. Under these assumptions the *Reynolds equation* applies.

For gas flows under the same conditions it is possible to derive a modified form of the Reynolds Equation, which uses the ideal gas law to eliminate the density from the equation system. This *modified Reynolds equation* can even be adapted to model the flow of rarefied gases.

Different terminology is used for thin-film flow in different fields of physics. In tribology the term *lubrication* is frequently used, especially when the fluid is a liquid.

In resonant MEMS devices, flow in the thin layer of gas separating a device from the substrate on which it is fabricated often provides significant *damping*. In this case there is usually a distinction between *squeeze-film damping*, when the direction of motion of the structure is predominantly perpendicular to the reference plane, and *slide-film damping* for motion predominantly parallel to the reference plane.

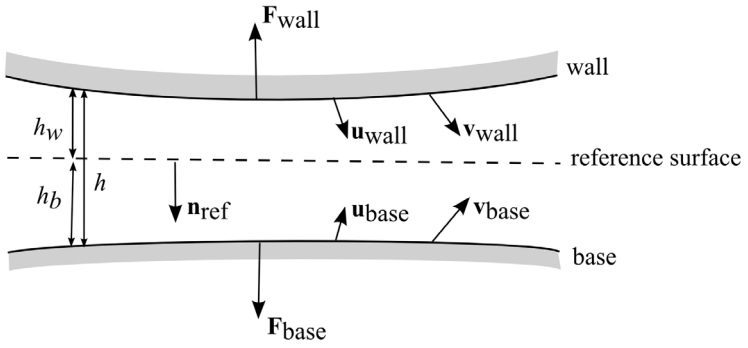


Figure 9-2: A typical configuration for thin-film flow. The reference surface with normal $\mathbf{n}_{\text{ref}}$ *sits in a narrow gap between a wall and base. The vector* $\mathbf{n}_{\text{ref}}$ *points into the base and out of the wall. The wall moves with a displacement* $\mathbf{u}_{\text{wall}}$ *and velocity* $\mathbf{v}_{\text{wall}}$ *from its initial position. Similarly the base moves from its initial position with displacement* $\mathbf{u}_{\text{base}}$ *and velocity* $\mathbf{v}_{\text{base}}$*. The compression of the fluid results in an excess pressure,* p_f*, above the reference pressure,* p_{ref}*, and a fluid velocity in the gap. At a point on the reference surface the average value of the fluid velocity along a line perpendicular to the surface is given by the in plane vector* $\mathbf{v}_{\text{ave}}$*. The motion of the fluid results in forces on the wall (*$\mathbf{F}_{\text{wall}}$*) and on the base (*$\mathbf{F}_{\text{base}}$*). The distance to the wall above the reference surface is* h_w *while the base resides a distance* h_b *below the reference surface. The total size of the gap is* $h = h_w + h_b$*. At a given time,* $h_w = h_{w1} - \mathbf{n}_{\text{ref}} \cdot \mathbf{u}_{\text{wall}}$ *and* $h_b = h_{b1} + \mathbf{n}_{\text{ref}}\mathbf{u}_{\text{base}}$*, where* h_{w1} *and* h_{b1} *are the initial distances to the wall and base, respectively.*

The Reynolds Equation

The equations of fluid flow in thin films are usually formulated on a reference surface in the Eulerian frame. Consider a cylinder, fixed with respect to a stationary reference surface, as shown in Figure 9-3.

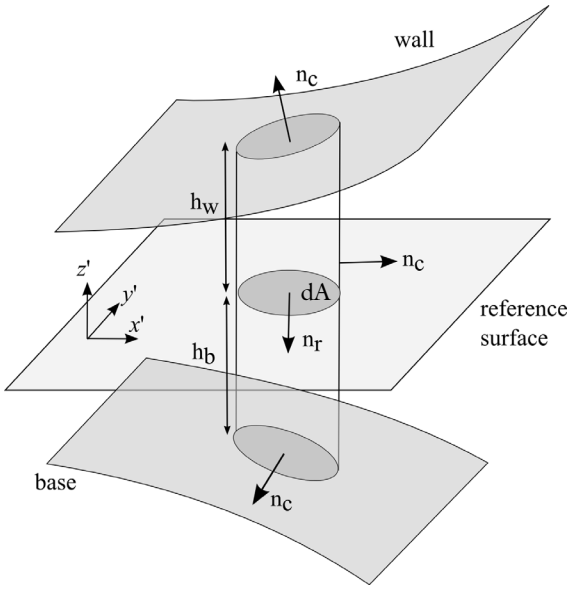


Figure 9-3: Reference cylinder, fixed with respect to the stationary reference surface, in a small gap between two surfaces (the wall and the base). The cylinder has outward normal, $\mathbf{n}_c$*. Its area, projected onto the reference surface, is dA.*

The cylinder is fixed with respect to the reference surface, but its height can change due to changes in the position of the base and the wall. Considering the flow in the reference plane, the rate at which mass accumulates within the reference cylinder is determined by the divergence of the mass flow field in the reference plane:

$$\frac{d}{dt}(\rho h) = -\nabla_t \cdot (\rho h \mathbf{v}_{\text{av}}) \tag{9-1}$$

where $h = h_w + h_b$ and the tangential velocity, $\mathbf{v}_{\text{av}}$, represents the mean velocity of the flow in the reference plane. Particular care must be taken with respect to the definition of h. The above equation applies if h is measured with respect to a fixed point on the reference surface as a function of time. The reference surface itself must be fixed in space and cannot deform as time progresses. Equations represented on the reference surface are described as Eulerian, that is they are defined in a frame that is fixed with respect to the motion of the fluid or of the body. Fluid flow problems are usually formulated in the Eulerian frame, and COMSOL Multiphysics adopts this convention in most of its fluid flow interfaces. It is useful to note that the Eulerian frame is usually

called the spatial frame within the COMSOL Multiphysics interface. When a structure deforms in COMSOL Multiphysics, the spatial frame changes shape.

The wall and the base can, and often do, move with respect to the reference surface. The wall and base are usually the surfaces of mechanical components which are deforming as a result of the pressure building up within the region of fluid flow. When describing the physics of a deforming solid, it is often convenient to work in the Lagrangian frame, which is fixed with respect to a small control volume of the solid. As the solid deforms, the Lagrangian frame moves along with the material contained within the control volume. Using the Lagrangian frame for describing structural deformation means that changes in the local density and material orientation as a result of the distortion of the control volume do not need to be accounted for by complicated transformations. In COMSOL Multiphysics, the Lagrangian frame, usually referred to as the material frame, is used for describing structural deformations. When a structure deforms in COMSOL Multiphysics, the material frame remains in the original configuration of the structure, and the deformation is accounted for by the underlying equations.

Because of the mixed Eulerian–Lagrangian approach adopted within COMSOL Multiphysics, particular care must be taken with the formulation of the Reynolds equation. Typically it is not desirable to represent the geometry of the thin film itself directly, because it is often much thinner than the other components in the model. The equations apply on a single surface in the model, the reference surface. The equations are added in the material frame (even though this frame is normally used in a Lagrangian approach) and manual transformations are added to the system to account for the fact that the structural equations also exist in the material frame, and employ a truly Lagrangian approach.

The situation encountered when both the wall and the base undergo a displacement is depicted in Figure 9-4. The Eulerian wall height changes from an initial value h_{w1} to a final value h_w. Similarly the base height changes from an initial value h_{b1} to h_b.

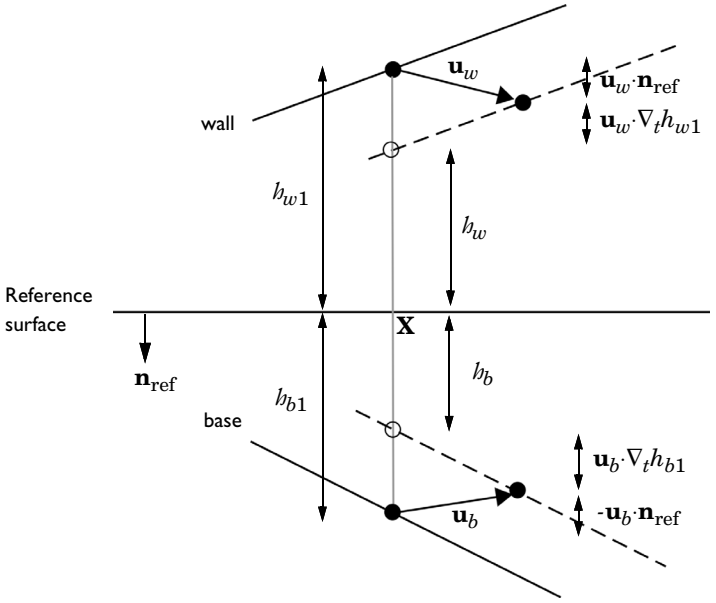


Figure 9-4: Diagram showing the displacement of the wall and the base with respect to the reference surface, and the corresponding change in the height of the channel.

From the figure it is clear that:

$$\begin{aligned} h_w &= h_{w1} - \mathbf{u}_w \cdot \mathbf{n}_{\text{ref}} - \mathbf{u}_w \cdot \nabla_t h_{w1} \\ h_b &= h_{b1} + \mathbf{u}_b \cdot \mathbf{n}_{\text{ref}} - \mathbf{u}_b \cdot \nabla_t h_{b1} \\ h &= h_w + h_b \end{aligned} \tag{9-2}$$

Similar corrections should be applied to the velocity of the wall if it is computed from the structural displacement. That is, the velocity should be modified by a term proportional to its spatial gradient. However, this correction term a second order term, and consequently it is usually negligible in practical circumstances. It is neglected in the Thin-Film Flow interface.

Consequently, provided that the definitions of the wall and base height from Equation 9-2 are used, the Reynolds equation takes the form:

$$\frac{\partial}{\partial t}(\rho h) + \nabla_t \cdot (h \rho \mathbf{v}_{\text{av}}) = 0 \tag{9-3}$$

When the **Compute implicit height change from wall velocity** checkbox and/or **Compute implicit height change from base velocity** checkbox are selected, the height changes due to the wall and/or base velocity are computed as,

$$\begin{aligned}\frac{\partial h_w}{\partial t} &= -\mathbf{v}_w \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_w \cdot \nabla_t h_{w1} \\ \frac{\partial h_b}{\partial t} &= \mathbf{v}_b \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_b \cdot \nabla_t h_{b1}\end{aligned} \tag{9-4}$$

The wall and base velocities effectively induce mass sources Q_w^{eff} and Q_b^{eff} which are added to the right-hand side of Equation 9-3, with,

$$\begin{aligned}Q_w^{\text{eff}} &= \rho(\mathbf{v}_w \cdot \mathbf{n}_{\text{ref}} + \mathbf{v}_w \cdot \nabla_t h_{w1}) \\ Q_b^{\text{eff}} &= -\rho(\mathbf{v}_b \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_b \cdot \nabla_t h_{b1})\end{aligned} \tag{9-5}$$

Flow Models

The Navier–Stokes equations can be nondimensionalized for a domain whose width (h_0) is much smaller than its lateral dimension(s) (l_0) (see Ref. 1 for a detailed discussion). When $\text{Re}(h_0/l_0)^2 << 1$, and terms of order $(h_0/l_0)^2$ and higher are

neglected, the Navier–Stokes equations reduce to a modified form of the Stokes equation, which must be considered in conjunction with the continuity relation.

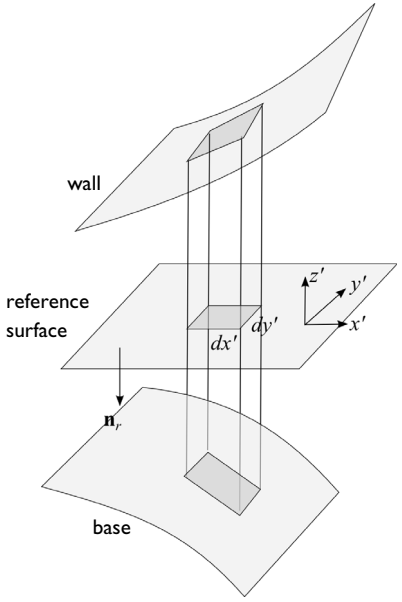


Figure 9-5: The coordinate system employed for the average flow velocity.

The equations are most conveniently expressed in a local coordinate system, in which x' and y' are tangent to the plane of the reference surface, and z' is perpendicular to the surface, as illustrated in Figure 9-5, which uses the coordinate system

$$\frac{\partial p_{\text{film}}}{\partial x'} = \frac{\partial}{\partial z'}\left(\mu \frac{\partial v_{x'}}{\partial z'}\right)$$

$$\frac{\partial p_{\text{film}}}{\partial y'} = \frac{\partial}{\partial z'}\left(\mu \frac{\partial v_{y'}}{\partial z'}\right)$$

$$\frac{\partial p_{\text{film}}}{\partial z'} = 0$$

where p_{film} is the pressure resulting from the fluid flow, μ is the fluid viscosity, and $(v_{x'},v_{y'})$ is the fluid velocity in the reference plane (which varies in the z' direction).

By making the assumption that the viscosity is constant through the film thickness, these equations can be integrated, yielding the in-plane velocity distributions. The following equations are derived:

$$\frac{\partial v_{x'}}{\partial z'} = \frac{z'}{\mu}\frac{\partial p_{\text{film}}}{\partial x'} + \frac{C_{1x'}}{\mu} \qquad \frac{\partial v_{y'}}{\partial z'} = \frac{z'}{\mu}\frac{\partial p_{\text{film}}}{\partial y'} + \frac{C_{1y'}}{\mu} \tag{9-6}$$

$$v_{x'} = \frac{z^2}{2\mu}\frac{\partial p_{\text{film}}}{\partial x'} + \frac{C_{1x'}z'}{\mu} + C_{2x'} \qquad v_{y'} = \frac{z^2}{2\mu}\frac{\partial p_{\text{film}}}{\partial y'} + \frac{C_{1y'}z'}{\mu} + C_{2y'} \tag{9-7}$$

The constants $C_{1x'}$, $C_{2x'}$, $C_{1y'}$, and $C_{2y'}$ are determined by the boundary conditions.

Equation 9-6 shows that the flow is a linear combination of laminar Poiseuille and Couette flows. The velocity profile is quadratic in form, as shown in Equation 9-7.

The average flow rate in the reference plane, $\mathbf{v}_{\text{av}}$, is given by

$$\mathbf{v}_{\text{av}} = \begin{bmatrix} \frac{1}{h}\int_{-h_b}^{h_w} v_{x'}dz' \\ \frac{1}{h}\int_{-h_b}^{h_w} v_{y'}dz' \end{bmatrix} = \begin{bmatrix} \frac{(h_w^2 - h_w h_b + h_b^2)}{6\mu}\frac{\partial p_{\text{film}}}{\partial x'} + \frac{h_w - h_b}{2\mu}C_{1x'} + C_{2x'} \\ \frac{(h_w^2 - h_w h_b + h_b^2)}{6\mu}\frac{\partial p_{\text{film}}}{\partial y'} + \frac{h_w - h_b}{2\mu}C_{1y'} + C_{2y'} \end{bmatrix}$$

The forces acting on the walls are determined by the normal component of the viscous stress tensor, τ, at the walls ($\tau\mathbf{n}$, where $\mathbf{n}$ is the normal that points out of the fluid domain). The viscous stress tensor takes the form

$$\tau = \mu(\nabla\mathbf{v} + (\nabla\mathbf{v}^T)) - p\mathbf{I} = \begin{bmatrix} -p_{\text{film}} + 2\mu\frac{\partial v_{x'}}{\partial x'} & \mu\left(\frac{\partial v_{y'}}{\partial x'} + \frac{\partial v_{x'}}{\partial y'}\right) & \mu\left(\frac{\partial v_{z'}}{\partial x'} + \frac{\partial v_{x'}}{\partial z'}\right) \\ \mu\left(\frac{\partial v_{x'}}{\partial y'} + \frac{\partial v_{y'}}{\partial x'}\right) & -p_{\text{film}} + 2\mu\frac{\partial v_{y'}}{\partial y'} & \mu\left(\frac{\partial v_z}{\partial y'} + \frac{\partial v_{y'}}{\partial z'}\right) \\ \mu\left(\frac{\partial v_{x'}}{\partial z'} + \frac{\partial v_{z'}}{\partial x'}\right) & \mu\left(\frac{\partial v_{y'}}{\partial z'} + \frac{\partial v_z}{\partial y'}\right) & -p_{\text{film}} + 2\mu\frac{\partial v_{z'}}{\partial z'} \end{bmatrix}$$

Neglecting the gradient terms, which are of order h_0/l_0, results in the simplified stress tensor

$$\tau \approx \begin{bmatrix} -p_{\text{film}} & 0 & \mu\dfrac{\partial v_{x'}}{\partial z'} \\ 0 & -p_{\text{film}} & \mu\dfrac{\partial v_{y'}}{\partial z'} \\ \mu\dfrac{\partial v_{x'}}{\partial z'} & \mu\dfrac{\partial v_{y'}}{\partial z'} & -p_{\text{film}} \end{bmatrix} \tag{9-8}$$

The components of the stress tensor can be expressed in terms of the velocity and pressure gradients using Equation 9-6. Note that the normals to both the wall and the base are parallel to the z' direction, to zeroth order in h_0/l_0. The forces acting on the base and the wall are therefore given by

$$f_w = \begin{bmatrix} \dfrac{h_w}{\mu}\dfrac{\partial p_{\text{film}}}{\partial x'} + \dfrac{C_{1x'}}{\mu} \\ \dfrac{h_w}{\mu}\dfrac{\partial p_{\text{film}}}{\partial y'} + \dfrac{C_{1y'}}{\mu} \\ p_{\text{film}} \end{bmatrix} \qquad f_b = \begin{bmatrix} \dfrac{h_b}{\mu}\dfrac{\partial p_{\text{film}}}{\partial x'} + \dfrac{C_{1x'}}{\mu} \\ \dfrac{h_b}{\mu}\dfrac{\partial p_{\text{film}}}{\partial y'} + \dfrac{C_{1y'}}{\mu} \\ -p_{\text{film}} \end{bmatrix}$$

GENERAL SLIP BOUNDARY CONDITION

Assuming a slip length of L_{sw} at the wall and a slip length of L_{sb} at the base, the general slip boundary conditions are given by

$$\begin{aligned} v_{x'}(z' = -h_b) - v_{x'}^b &= \frac{L_{sb}}{\mu}\tau_{z'x'}(z' = -h_b) = L_{sb}\frac{\partial v_{x'}}{\partial z'}(z' = -h_b) \\ v_{y'}(z' = -h_b) - v_{y'}^b &= \frac{L_{sb}}{\mu}\tau_{z'y'}(z' = -h_b) = L_{sb}\frac{\partial v_{y'}}{\partial z'}(z' = -h_b) \\ v_{x'}(z' = h_w) - v_{x'}^w &= -\frac{L_{sw}}{\mu}\tau_{z'x'}(z' = h_w) = -L_{sw}\frac{\partial v_{x'}}{\partial z'}(z' = h_w) \\ v_{y'}(z' = h_w) - v_{y'}^w &= -\frac{L_{sw}}{\mu}\tau_{z'y'}(z' = h_w) = -L_{sw}\frac{\partial v_{y'}}{\partial z'}(z' = h_w) \end{aligned} \tag{9-9}$$

For nonidentical slip lengths the constants $C_{1x'}$, $C_{2x'}$, $C_{1y'}$, and $C_{2y'}$ take the following values:

$$C_{1x'} = \frac{\mu(v_{x'}^w - v_{x'}^b)}{h + L_{sw} + L_{sb}} - \frac{h_b^2 - h_w^2 - 2L_{sw}h_w + 2L_{sb}h_b}{2(h + L_{sb} + L_{sw})}\frac{\partial p_{\text{film}}}{\partial x'}$$

$$C_{2x'} = \frac{v_{x'}^w(h_b + L_{sb}) + v_{x'}^b(h_w + L_{sw})}{h + L_{sw} + L_{sb}}$$

$$-\frac{h_w^2(h_b + L_{sb}) + h_b^2(h_w + L_{sw}) + 2h_w h_b(L_{sw} + L_{sb}) + 2hL_{sw}L_{sb}}{2(h + L_{sw} + L_{sb})\mu}\frac{\partial p_{\text{film}}}{\partial x'}$$

$$C_{1y'} = \frac{\mu(v_{y'}^w - v_{y'}^b)}{h + L_{sw} + L_{sb}} - \frac{h_b^2 - h_w^2 - 2L_{sw}h_w + 2L_{sb}h_b}{2(h + L_{sw} + L_{sb})}\frac{\partial p_{\text{film}}}{\partial y'}$$

$$C_{2y'} = \frac{v_{y'}^w(h_b + L_{sb}) + v_{y'}^b(h_w + L_{sw})}{h + L_{sw} + L_{sb}}$$

$$-\frac{h_w^2(h_b + L_{sb}) + h_b^2(h_w + L_{sw}) + 2h_w h_b(L_{sw} + L_{sb}) + 2hL_{sw}L_{sb}}{2(h + L_{sw} + L_{sb})\mu}\frac{\partial p_{\text{film}}}{\partial y'}$$

The average flow rate becomes

$$\mathbf{v}_{\text{av}} = \begin{bmatrix} \frac{h(v_{x'}^w + v_{x'}^b) + 2(L_{sw}v_{x'}^w + L_{sb}v_{x'}^b)}{2(h + L_{sw} + L_{sb})} - \frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})}\frac{\partial p_{\text{film}}}{\partial x'} \\ \frac{h(v_{y'}^w + v_{y'}^b) + 2(L_{sw}v_{y'}^w + L_{sb}v_{y'}^b)}{2(h + L_{sw} + L_{sb})} - \frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})}\frac{\partial p_{\text{film}}}{\partial y'} \end{bmatrix}$$

which can be expressed in vector notation as

$$\mathbf{v}_{\text{av}} = \frac{1}{2(h + L_{sw} + L_{sb})}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r^T)((h + 2L_{sw})\mathbf{v}_w + (h + 2L_{sb})\mathbf{v}_b)$$

$$-\frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})}\nabla_t p_{\text{film}}$$

The above equation can be written on the form

$$\mathbf{v}_{\text{av}} = \mathbf{v}_{\text{av},c} - v_{\text{av},p}\nabla_t p_{\text{film}} \tag{9-10}$$

where $\mathbf{v}_{\text{av},c}$ is a term associated with Couette flow, and $v_{\text{av},p}$ is a coefficient associated with Poiseuille flow (see Table 9-2 below).

The forces acting on the two boundaries are given by

$$\mathbf{f}_w = \begin{bmatrix} -\dfrac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})}\dfrac{\partial p_{\text{film}}}{\partial x'} + \dfrac{(v_{x'}^b - v_{x'}^w)\mu}{(h+L_{sw}+L_{sb})} \\ -\dfrac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})}\dfrac{\partial p_{\text{film}}}{\partial y'} + \dfrac{(v_{y'}^b - v_{y'}^w)\mu}{(h+L_{sw}+L_{sb})} \\ p_{\text{film}} \end{bmatrix}$$

$$\mathbf{f}_b = \begin{bmatrix} -\dfrac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})}\dfrac{\partial p_{\text{film}}}{\partial x'} + \dfrac{(v_{x'}^w - v_{x'}^b)\mu}{(h+L_{sw}+L_{sb})} \\ -\dfrac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})}\dfrac{\partial p_{\text{film}}}{\partial y'} + \dfrac{(v_{y'}^w - v_{y'}^b)\mu}{(h+L_{sw}+L_{sb})} \\ -p_{\text{film}} \end{bmatrix} \quad (9\text{-}11)$$

Note that the z' direction corresponds to the $-\mathbf{n}_r$ direction. The x' and y' directions correspond to the two tangent vectors in the plane. Using vector notation the forces become:

$$\mathbf{f}_w = -\frac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})}\nabla_t p_{\text{film}} + \frac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b-\mathbf{v}^w) + p_{\text{film}}\mathbf{n}_w$$

$$\mathbf{f}_b = -\frac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})}\nabla_t p_{\text{film}} + \frac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w-\mathbf{v}^b) + p_{\text{film}}\mathbf{n}_b$$

In Equation 9-11 it is assumed that $\mathbf{n}_w = -\mathbf{n}_r$ and $\mathbf{n}_b = \mathbf{n}_r$. In COMSOL Multiphysics, the accuracy of the force terms is improved slightly over the usual approximation (which neglects the slope of the wall and base as it is of order h_0/l_0) by using the following equations for $\mathbf{n}_w$ and $\mathbf{n}_b$:

$$\mathbf{n}_w = (-\mathbf{n}_r - \nabla_t h_w)$$

$$\mathbf{n}_b = (\mathbf{n}_r - \nabla_t h_w)$$

These definitions are derived from Equation 9-6 and Equation 9-7 and include the additional area that the pressure acts on as a result of the wall slope.

The force terms can be written on vector notation:

$$\begin{aligned} \mathbf{f}_w &= -f_{w,p}\nabla_t p_{\text{film}} + \mathbf{f}_{w,c} \\ \mathbf{f}_b &= -f_{b,p}\nabla_t p_{\text{film}} + \mathbf{f}_{b,c} \end{aligned} \quad (9\text{-}12)$$

where $f_{w,p}$ is the Poiseuille coefficient for the force on the wall, and $\mathbf{f}_{w,c}$ incorporates the Couette and normal forces (due to the pressure) on the wall. Similarly, $f_{b,p}$ is the Poiseuille coefficient for the force on the base, and $\mathbf{f}_{b,c}$ incorporates the Couette and normal forces (due to the pressure) on the base.

The cases of identical slip length and no slip are limiting cases of the formulas derived above. The main results are summarized in Table 9-2, where the constants defined in Equation 9-10 and Equation 9-12 are used.

TABLE 9-2: EQUATION VARIABLES FOR VARIOUS FLOW MODELS.

VARIABLE	DEFINITION
General Slip Flow Model	
$\mathbf{v}_{\mathrm{av},c}$	$\frac{1}{2(h+L_{sw}+L_{sb})}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)((h+2L_{sb})\mathbf{v}_w+(h+2L_{sw})\mathbf{v}_b)$
$v_{\mathrm{av},p}$	$\frac{h(h^2+4h(L_{sw}+L_{sb})+12L_{sb}L_{sw})}{12\mu(h+L_{sw}+L_{sb})}$
$\mathbf{f}_{w,c}$	$\frac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b-\mathbf{v}^w)+p_{\mathrm{film}}\mathbf{n}_w$
$f_{w,p}$	$\frac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})}$
$\mathbf{f}_{b,c}$	$\frac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w-\mathbf{v}^b)+p_{\mathrm{film}}\mathbf{n}_b$
$f_{b,p}$	$\frac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})}$
Equal Slip Lengths Flow Model Lsw=Lsb=L	
$\mathbf{v}_{\mathrm{av},c}$	$\frac{1}{2}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}_w+\mathbf{v}_b)$
$v_{\mathrm{av},p}$	$(h^2+6L_sh)/(12\mu)$
$\mathbf{f}_{w,c}$	$\frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b-\mathbf{v}^w)+p_{\mathrm{film}}\mathbf{n}_w$
$f_{w,p}$	$h/2$
$\mathbf{f}_{b,c}$	$\frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w-\mathbf{v}^b)+p_{\mathrm{film}}\mathbf{n}_b$
$f_{b,p}$	$h/2$

TABLE 9-2: EQUATION VARIABLES FOR VARIOUS FLOW MODELS.

VARIABLE	DEFINITION
Nonslip Flow Model Lsw=Lsb=0	
$\mathbf{v}_{\mathrm{av},c}$	$\frac{1}{2}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}_w+\mathbf{v}_b)$
$v_{\mathrm{av},p}$	$h^2/(12\mu)$
$\mathbf{f}_{w,c}$	$\frac{\mu}{h}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b-\mathbf{v}^w)+p_{\mathrm{film}}\mathbf{n}_w$
$f_{w,p}$	$h/2$
$\mathbf{f}_{b,c}$	$\frac{\mu}{h}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w-\mathbf{v}^b)+p_{\mathrm{film}}\mathbf{n}_b$
$f_{b,p}$	$h/2$

The Modified Reynolds Equation — Gas Flow

Thin-film gas flow is often isothermal, and in many cases the ideal gas law can be assumed. The ideal gas assumption relates the gas density to the pressure as

$$\rho = \frac{M_n}{RT_0}p_A$$

here, T_0 is the (constant) temperature of the gas, M_n is the molar mass, and R is the universal gas constant. The total gas pressure, $p_A = p_{\mathrm{ref}} + p_{\mathrm{film}}$, is written in terms of the reference pressure level p_{ref} and the pressure developed in the thin-film flow, p_{film}. Substituting this density into Equation 9-3 and dividing it by M_n/RT_0 results in the modified Reynolds equation for ideal (isothermal) gases:

$$\frac{\partial}{\partial t}(p_A h)+\nabla_t\cdot(hp_A\mathbf{v}_{\mathrm{av}}) = 0 \qquad (9\text{-}13)$$

The average flow rate and the forces acting on the walls are computed in the same manner as for the standard Reynolds equation.

When the **Compute implicit height change from wall velocity** checkbox and/or **Compute implicit height change from base velocity** checkbox are selected, the height changes due to the wall and/or base velocity are computed as,

$$\frac{\partial h_w}{\partial t} = -\mathbf{v}_w \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_w \cdot \nabla_t h_{w1}$$
$$\frac{\partial h_b}{\partial t} = \mathbf{v}_b \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_b \cdot \nabla_t h_{b1} \quad (9\text{-}14)$$

The wall and base velocities effectively induce mass sources Q_w^{eff} and Q_b^{eff} which are added to the right-hand side of Equation 9-13, with,

$$Q_w^{\text{eff}} = p_A(\mathbf{v}_w \cdot \mathbf{n}_{\text{ref}} + \mathbf{v}_w \cdot \nabla_t h_{w1})$$
$$Q_b^{\text{eff}} = -p_A(\mathbf{v}_b \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_b \cdot \nabla_t h_{b1}) \quad (9\text{-}15)$$

SLIP BOUNDARY CONDITION FOR GASES

For a gas, the slip length is often expressed using the *mean free path*, λ, and a *tangential momentum accommodation* coefficient, α. The following definition of the mean free path is used in the Thin-Film Flow interfaces:

$$\lambda = \frac{\mu}{p}\left(\frac{\pi RT}{2M_n}\right)^{\frac{1}{2}}$$

where μ is the gas viscosity, p is the gas pressure, R is the molar gas constant, T is the temperature, and M_n is the molar mass of the gas. This definition differs from the equivalent free path in Ref. 3 by a factor $\sqrt{\pi}/2$.

The slip length is then defined as

$$L_s = \lambda\left(\frac{2-\alpha}{\alpha}\right)$$

Values for the a *tangential momentum accommodation* coefficient, α for various gas-surface combinations are given in Ref. 2.

Flow Models for Rarefied Gases

For gases at low pressure, the ratio of the gas mean free path, λ, to the gap size (known as the Knudsen number: $\text{Kn} = \lambda/h$) grows. For Knudsen numbers greater than 0.1, the gas cannot be treated using the continuum Navier–Stokes equations, and the Boltzmann equation must be solved instead.

At steady state, the solutions to the linearized Boltzmann equation for isothermal flow in a narrow gap between parallel plates can be expressed as a combination of Poiseuille

and Couette flows. This is analogous to the solutions of the Navier–Stokes equations in the limit of small h_0/l_0.

Provided that the wall and base surfaces are identical (which is normally the case in many practical applications), the Couette contribution to the bulk fluid velocity is unchanged (it remains the mean of the wall and base velocities for identical surfaces).

The Poiseuille contribution to the flow is more complicated for rarefied gases. A practical approach, pioneered by Fukui and Kaneko (Ref. 4) is to solve the linearized Boltzmann BGK equation over a range of Knudsen numbers and to provide an empirical fit to the flow. This results in the following form for the average flow velocity:

$$\mathbf{v}_{\text{av}} = \frac{1}{2}(\mathbf{I} - \mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}_w + \mathbf{v}_b) - \frac{h^2}{12\mu_{\text{eff}}}\nabla_t p$$
$$\mu_{\text{eff}} = \frac{\mu}{Q(\text{Kn}, \alpha_w, \alpha_b)} \tag{9-16}$$

where $Q(\text{Kn}, \alpha_w, \alpha_b)$ is a nondimensional function of the Knudsen number (Kn), and the *tangential momentum accommodation* coefficients at the wall and base (α_w and α_b).The function $Q(\text{Kn}, \alpha_w, \alpha_b)$ is obtained by solving the linearized Boltzmann BGK equation for steady Poiseuille flow with a range of Knudsen numbers and slip coefficients. This approach assumes that stationary solutions of the Boltzmann equation apply inside the gap, that is, that the flow can be treated as quasi static.

In Ref. 5 there is data for $Q(\text{Kn}, \alpha_w, \alpha_b)$ in the case where $\alpha_w = \alpha_b$, which was subsequently fitted to different empirical formulas by Veijola and others (Ref. 6). Note also that additional and more accurate data is available in Ref. 7. In Ref. 6 there are two empirical formulas, which apply under different circumstances with various degrees of accuracy:

- $\alpha_w = \alpha_b = 1$ (available as the option **Rarefied-total accommodation**):

  $$Q(\text{Kn},1,1) = 1 + 9{,}638\text{Kn}^{1{,}159}$$

  which is accurate to within 5% in the range $0 < \text{Kn} < 880$.
- $\alpha_w = \alpha_b = \alpha$ (available as the option **Rarefied-general accommodation**):

$$Q(\mathrm{Kn},\alpha,\alpha) = \frac{6\tilde{Q}(D,\alpha)}{D} \qquad D = \frac{\sqrt{\pi}}{2\mathrm{Kn}}$$

$$\tilde{Q}(D,\alpha) = \frac{D}{6} + \frac{1}{\alpha^{1.34}\sqrt{\pi}}\ln\left(\frac{1}{D}+4.1\right) + \frac{\alpha}{6.4} + \frac{1.3(1-\alpha)}{1+0.08D^{1.83}} + \frac{0.64\alpha D^{0.17}}{1+1.12D^{0.72}}$$

which is accurate to within 1% in the ranges $0.7 < \alpha < 1$, and $0.01 < \mathrm{Kn} < 88$.

Both of these empirical models are available as flow models. Additionally, a user defined **relative flow rate function** Q can be defined for Equation 9-16, which could be based on an interpolation data as described in Ref. 7. Data on the tangential momentum accommodation coefficients for various gas-surface combinations is also available in Ref. 2.

In many applications the forces acting on the wall and base are important. The pressure in the gas can be computed correctly by solving Equations 9-13 and 9-16. However, this approach provides only the normal component of the traction acting on the wall and base. To obtain the shear forces, the approach adopted by Torczynski and Gallis (Ref. 8) is used. They produced an empirical expression for the shear force that has the correct behavior in the free molecular flow and continuum limits as well as in the limits for the accommodation coefficient. Torczynski and Gallis solve the problem of pure Couette flow and derive an empirical function for the slip length that predicts the correct forces for the flow in the gap in several limiting cases. Their empirical expression for the slip length is given by

$$L_s = \frac{(2-\alpha)}{\alpha}\lambda\left(1+\frac{d_1\alpha}{1+d_2\mathrm{Kn}}\right) \tag{9-17}$$

where $d_1 \approx 0.15$ and $d_2 \approx 0.59$. In principle d_1 and d_2 are variables themselves, but they were found to be constant to within the accuracy of the DSMC experiments used to derive their values.

Equation 9-10 gives the following expressions for the shear forces on the wall and base for pure Couette flow:

$$\mathbf{f}_w^{\mathrm{shear}} = \frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b-\mathbf{v}^w)$$

$$\mathbf{f}_b^{\mathrm{shear}} = \frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w-\mathbf{v}^b)$$

where L_s is taken from Equation 9-17.

A general flow incorporates both Poiseuille and Couette terms. Assuming that the Poiseuille and Couette flows can be superposed, the forces become

$$\begin{aligned}\mathbf{f}_w &= -\frac{h}{2}\nabla_t p + \frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b-\mathbf{v}^w) - p\mathbf{n}_r \\ \mathbf{f}_b &= -\frac{h}{2}\nabla_t p + \frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w-\mathbf{v}^b) + p\mathbf{n}_r\end{aligned} \tag{9-18}$$

here L_s is derived from Equation 9-17 and p is obtained by solving Equation 9-13 with Equation 9-16. Strictly speaking, Torczynski and Gallis' results apply for Couette flow only, and were derived for a more general variable-soft-sphere gas rather than for the linearized BGK equations. From a practical perspective, it seems likely that solutions of the linearized BGK equations would also be fitted by these expressions, and in that case it could be possible to combine the forces using superposition. In the absence of a detailed proof, Equation 9-18 is not the default option for the force model, but it is available as an additional option.

Both Ref. 6 and Ref. 7 provide data for the relative flow rate $Q(\mathrm{Kn}, \sigma_{sw}, \sigma_{sb})$ in specific cases where the wall and base have different accommodation coefficients. Since no details on how to compute the forces acting on the walls for highly rarefied gases were published, these models are not currently supported in COMSOL Multiphysics.

Frequency-Domain Formulation

In the frequency domain it is necessary to make additional simplifications to the equation system to produce a fully linearized equation set. In the general case, the physical quantities in the Reynolds and flow equations take the form:

$$h_w = h_{w1} + \tilde{h}_w \qquad h_b = h_{b1} + \tilde{h}_b \qquad h = h_{w1} + h_{b1} + \tilde{h}_w + \tilde{h}_b = h_1 + \tilde{h}$$
$$p_{\text{film}} = \tilde{p}_{\text{film}} \qquad p_A = p_{\text{ref}} + \tilde{p}_{\text{film}}$$
$$\mathbf{v}_w = \tilde{\mathbf{v}}_w \qquad \mathbf{v}_b = \tilde{\mathbf{v}}_b$$

Here the tilde denotes a harmonically varying component. The components marked with the subscript 1 are static offsets to the harmonic terms. In order to linearize the equation system, it is necessary to assume that the offsets are much larger than the harmonic perturbation. This means that the harmonically varying pressures induced by the flow should be significantly smaller than the ambient pressure, and the harmonic

changes in the gap size due to the wall and base displacements should be significantly less than the gap height itself. Given these assumptions, the average fluid velocity can also be written on the form

$$\mathbf{v}_{\text{av}} = \tilde{\mathbf{v}}_{\text{av}}$$

since in general both the Couette and Poiseuille terms vary harmonically to first-order accuracy.

Substituting these terms into the Reynolds equation gives

$$\frac{\partial}{\partial t}(\rho(h_1 + \tilde{h})) + \nabla_t \cdot (\rho(h_1 + \tilde{h})\tilde{\mathbf{v}}_{\text{av}}) = 0$$

In the frequency domain, the total absolute pressure p_A is set to the reference pressure p_{ref} because the deviation from the reference pressure p_{film} in this case represents an oscillating component and cannot be added to the pressure in a straightforward manner.The density ρ is defined as a function of p_A and does not contain the small harmonic component. The products of small harmonic terms result in second-order effects (at double the frequency of interest) and can be neglected provided the harmonic terms are much smaller than the static terms. The Reynolds equation therefore simplifies to

$$\rho\frac{\partial}{\partial t}(\tilde{h}) + \nabla_t \cdot (\rho h_1 \tilde{\mathbf{v}}_{\text{av}}) = 0$$

Note that

$$\frac{\partial}{\partial t}(\tilde{h}) = \tilde{\mathbf{v}}_b \cdot \mathbf{n}_{\text{ref}} - \tilde{\mathbf{v}}_w \cdot \mathbf{n}_{\text{ref}} - \tilde{\mathbf{v}}_b \cdot \nabla_t h_{b1} - \tilde{\mathbf{v}}_w \cdot \nabla_t h_{w1} \tag{9-19}$$

So the following result holds:

$$\rho(\tilde{\mathbf{v}}_b \cdot \mathbf{n}_{\text{ref}} - \tilde{\mathbf{v}}_w \cdot \mathbf{n}_{\text{ref}} - \tilde{\mathbf{v}}_b \cdot \nabla_t h_{b1} - \tilde{\mathbf{v}}_w \cdot \nabla_t h_{w1}) + \nabla_t \cdot (\rho h_1 \tilde{\mathbf{v}}_{\text{av}}) = 0 \tag{9-20}$$

Dropping the tildes leads to the form of the equation shown in the equation display:

$$\rho(\mathbf{v}_b \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_w \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_w \cdot \nabla_t h_{w1} - \mathbf{v}_b \cdot \nabla_t h_{b1}) + \nabla_t \cdot (\rho h_1 \mathbf{v}_{\text{av}}) = 0$$

The modified Reynolds equation takes the following form:

$$\frac{\partial}{\partial t}((p_{\text{ref}} + \tilde{p_{\text{film}}})(h_1 + \tilde{h})) + \nabla_t \cdot ((p_{\text{ref}} + \tilde{p_{\text{film}}})(h_1 + \tilde{h})\tilde{\mathbf{v}}_{\text{av}}) = 0 \tag{9-21}$$

Linearizing Equation 9-21 gives

$$p_{\text{ref}}\frac{\partial}{\partial t}\tilde{h} + h_1\frac{\partial}{\partial t}\tilde{p}_{\text{film}} + \nabla_t \cdot (p_{\text{ref}} h_1 \tilde{\mathbf{v}}_{\text{av}}) = 0$$

Equation 9-19 can be used to substitute for the time derivative of the harmonic component of h in the above equation, yielding

$$\begin{aligned} p_{\text{ref}}(\tilde{\mathbf{v}}_b \cdot \mathbf{n}_{\text{ref}} - \tilde{\mathbf{v}}_w \cdot \mathbf{n}_{\text{ref}} - \tilde{\mathbf{v}}_b \cdot \nabla_t h_{b1} - \tilde{\mathbf{v}}_w \cdot \nabla_t h_{w1}) \\ + h_1\frac{\partial}{\partial t}(\tilde{p}_{\text{film}}) + \nabla_t \cdot (p_{\text{ref}} h_1 \tilde{\mathbf{v}}_{\text{av}}) = 0 \end{aligned} \tag{9-22}$$

Dropping the tildes and using complex notation to express the time derivative of p_{film} gives:

$$\begin{aligned} p_{\text{ref}}(\mathbf{v}_b \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_w \cdot \mathbf{n}_{\text{ref}} - \mathbf{v}_w \cdot \nabla_t h_{w1} - \mathbf{v}_b \cdot \nabla_t h_{b1}) \\ + i\omega h_1 p_{\text{film}} + \nabla_t \cdot (p_{\text{ref}} h_1 \mathbf{v}_{\text{av}}) = 0 \end{aligned}$$

Equation 9-20 and Equation 9-22 are used as the basis for the frequency domain formulation in the Thin-Film Flow interfaces. It is important to note that these equations are independent of the harmonic components of the displacement, since those terms lead to second-order contributions to the frequency-domain response (that is, they produce a response proportional to the square of the harmonic term, which results in a signal at twice the driving frequency).

Since the frequency domain results do not depend on the variation in the displacement, the additional displacement setting has no effect on the solution in a frequency-domain problem (unless the velocity is computed from it by selecting **Calculate from wall displacement** or **Calculate from base displacement** in the wall and base velocity settings, respectively). This is reflected in the equations given above (and in the equation display in the physics interface) but can be nonintuitive, particularly when setting up a model that is coupled with a structural analysis. If the velocity of both the wall and the base is set to zero, then in the frequency domain there is no response.

Boundary Conditions

The boundary conditions constrain the flow into the system by either prescribing a fluid velocity or constrain the pressure on the boundary. The **Border flow** option allows to specify the value of the pressure gradient in the normal direction such that

$$-\mathbf{n} \cdot \nabla p = \Gamma$$

The **Border flow type** selection list allows four ways to specify the value of Γ:

- The two **Acoustic elongation** options assume a linear gradient in the pressure outside the domain away from the boundary. The pressure gradient is calculated by dividing the pressure at the boundary, p_{film}, by an elongation length, ΔL, such that

  $$-\mathbf{n} \cdot \nabla p = \frac{p_{\text{film}}}{\Delta L}$$

  The elongation length ΔL can either be specified as an absolute length or as a relative elongation of the width.
- The **Out-of-plane motion** option calculates the pressure gradient at the boundary using a model described in Ref. 9. This model is suitable for including the effects of gas damping when the thin-film is subjected to out-of-plane motion of the walls or base (for example, when a microbeam is oscillating above an extended surface). When this option is selected, the pressure gradient is defined according to the coefficients ζ, η, and χ:

  $$-\mathbf{n} \cdot \nabla p = \zeta \frac{12\mu U}{\eta h^2}\left(1 + \chi \frac{6\Lambda}{h}\right)^{-1} + \frac{p - p_\infty}{\eta h^2}$$

  where U is the out-of-plane velocity, Λ is the slip length at the walls, and p_∞ is the ambient pressure far away from the domain.
- The **User defined** option allows to enter values or expressions for the normal pressure gradient.

Cavitation

Several types of cavitation can occur in thin film flow. When the flow pressure drops below the ambient pressure, the air and other gases dissolved within the fluid are released. This phenomenon, characteristic of loaded bearings, is known as cavitation or gaseous cavitation. In some cases involving high frequency varying loads, as in internal combustion engines, the pressure might drop below the fluid vapor pressure,

which is lower than the ambient pressure. In this case, bubbles are formed by rapid evaporation or boiling. This phenomenon is known as vapor cavitation. The cavitation feature in COMSOL Multiphysics is designed to address gaseous cavitation.

The implementation of the cavitation feature is based on a modified version of the Elrod's algorithm (Ref. 10 and Ref. 11). This algorithm automatically predicts film rupture and reformation in bearings, and it offers a reasonable compromise between accuracy and practicality. It is applicable to heavily and moderately loaded bearings but it is not suitable when surface tension plays an important role.

Elrod and Adam's algorithm is based on the JFO cavitation theory, a widely accepted theory developed by Jakobsson (Ref. 12), Floberg (Ref. 13 and Ref. 14), and Olsson (Ref. 15). The JFO theory divides the flow in two regions:

- A full-film region where the pressure varies but is limited from below by the cavitation pressure.
- A cavitation region where only part of the volume is occupied by the fluid. Because of the presence of the gas in the void fraction, the pressure in this region is assumed to be constant and equal to the cavitation pressure.

Elrod and Adams derived a general form of the Reynolds equation, Equation 9-1, by introducing a switch function, g, equal to 1 in the full film region and 0 in the cavitation region. This switch function allows for solving a single equation for both the full film and the cavitation region and leads to a modified version of Equation 9-10:

$$\mathbf{v}_{\mathrm{av}} = \mathbf{v}_{\mathrm{av},c} - g v_{\mathrm{av},p} \nabla_t p_{\mathrm{film}}$$

where the second and third terms on the left-hand side correspond to the average Couette and average Poiseuille velocities, respectively. This switch function sets the average Poiseuille velocity to zero in the cavitation region.

Because the average Poiseuille velocity is set to zero in the cavitation region, the density needs to be a function of the pressure variable and is defined as

$$\rho = \rho_c e^{\beta p_f}$$

where β is the compressibility, and ρ_c is the density at the cavitation pressure. A density that is not pressure dependent would lead to empty equations in the cavitation region since the pressure variable p_{film} would no longer be present in the governing equations.

A variable θ can be defined, given by

$$\theta = \frac{\rho}{\rho_c}$$

In the cavitation region ($\theta < 1$), the variable θ represents the fractional film content.

NOTE ABOUT RESULTS POSTPROCESSING

While the pressure is constant and equal to the cavitation pressure in the cavitation region, the computed pressure is negative in this region. The value of this negative pressure can be physically be interpreted as the volume fraction of fluid in the cavitation region. The actual or physical pressure, available in the postprocessing section as `tff.p`, is equal to the computed pressure in the full film region ($\theta \geq 1$) and equal to the cavitation pressure in the cavitation region ($\theta < 1$).

References for the Thin-Film Flow Interfaces

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10

Shallow Water Interface

The physics interface described in this section is found under the **Shallow Water Equations** branch ( ).

In this chapter

- The Shallow Water Equations, Time Explicit Interface
- Theory for the Shallow Water Equations Interface

The Shallow Water Equations, Time Explicit Interface

In this section:

- The Shallow Water Equations, Time Explicit Interface
- Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface

Theory for the Shallow Water Equations Interface

The Shallow Water Equations, Time Explicit Interface

The **Shallow Water Equations, Time Explicit (swe)** interface ( ), found under the **Shallow Water Equations** branch ( ) when adding a physics interface, is used to solve the Shallow Water equations in a 1D or 2D geometry. These equations model the flow of a free surface in a fluid under the assumption that the horizontal scale is much greater than the vertical length scale. They are frequently used for modeling both oceanographic and atmospheric fluid flow. Models of such systems can be used to predict areas affected by pollution, coastal erosion, and polar ice-cap melting, provided the fluid layer is shallow enough.

Comprehensive modeling of such phenomena using physical descriptions such as the Navier–Stokes equations can often be problematic, due to the scale of the modeling domains as well as the resolution of free surfaces. The shallow water equations, of which there are a number of representations, provide an easier description of such phenomena.

A typical configuration for the flow of fluid in a shallow layer is shown in Figure 10-1.This physics interface approximates free surface problems where the thickness h of the fluid layer, or water depth, is small compared to the lateral dimensions of the geometry. The lower boundary of the fluid is treated as a nonpenetrable wall and has a height $h_b(x, y)$ over a reference xy-plane placed at $z = 0$. The topography of the bottom is assumed constant in time. Using the shallow water equations, the water depth h and water flux $\mathbf{q}$ are computed in a reduced dimension

of the problem. Free surface problems that would require a 3D geometry when modeled with the Navier–Stokes equations can be modeled in 2D instead. 2D problems can also be reduced to 1D.

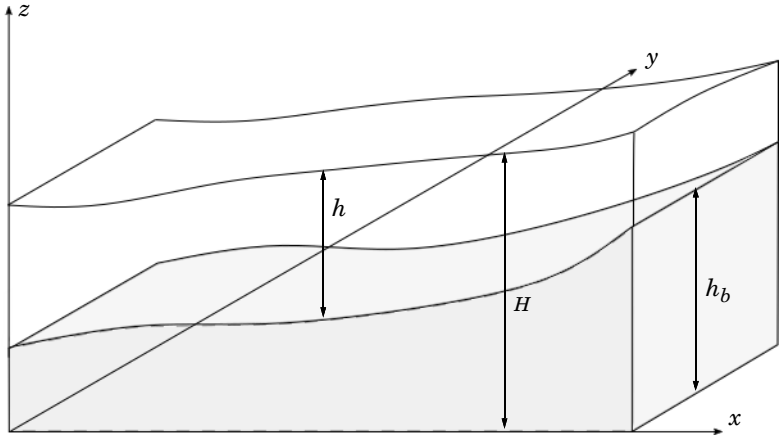

Figure 10-1: An example illustrating a typical configuration for shallow water equations. A water layer of thickness h *flows over a nonflat bottom with topography represented by* h_b*. The total height of the free surface over the reference* xy *plane at* $z = 0$ *is represented by* H*. The gravity points downward (–*z *direction) and gives rise to a hydrostatic pressure ranging from* 0 atm *at the free surface to a value of* $g\rho h$ *at the bottom.*

Since the physics interface supports **Nodal discontinuous Lagrange** functions with **Constant Element order** for the discretization of the **Dependent variables**, the spatial derivatives are zero. Hence, the physics interface cannot be used in conjunction with **Moving Mesh** functionality.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Domain Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, you can add other nodes that implement, for example, boundary conditions. You can also right-click **Shallow Water Equations, Time Explicit** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to

different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `swe`.

PHYSICAL MODEL

Select a value for **Acceleration of gravity** (SI unit m/s). The default value is g_{const}. It should be a global quantity.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog. Normally these settings do not need to be changed.

Select the **CFL number**. This CFL number will be used when defining the **Cell time scale expression** `swe.wtc` used in the **Time-Explicit Solver** if the **Time stepping** is set to **From expressions**. Note that the method will be unstable for CFL numbers larger than 1.

In the *COMSOL Multiphysics Reference Manual*:

- References for the Solution Operation Nodes and Solvers

DISCRETIZATION

The Shallow Water Equations, Time Explicit interface uses **Nodal discontinuous Lagrange** functions with **Constant Element order**.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Water depth** h (SI unit: m) and the **Water flux** $\mathbf{q}$ (SI unit: m^2 /s). The names can be changed but the names of fields and dependent variables must be unique within a component.

- Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface
- Theory for the Shallow Water Equations Interface

- *Dam Breaking on a Column, Shallow Water Equations*: Application Library path **CFD_Module/Shallow_Water_Equations/dam_break_column_sw**
- *Tsunami Runup onto a Complex 3D Beach, Monai Valley*: Application Library path **CFD_Module/Shallow_Water_Equations/monai_runup**

Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface

For the Shallow Water Equations interface, the following domain, boundary, edge, point, and pair nodes (listed in alphabetical order) are described in this section:

- Domain Properties
- Domain Source
- Initial Values
- Inlet
- Interior Wall
- Outlet
- Symmetry
- Wall
- Water Source

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Domain Properties

Use the **Domain Properties** node to set the bottom topography and material properties.

BOTTOM TOPOGRAPHY

The **Bottom height** (SI unit: m) is defined as a user defined expression. It can depend on the geometry coordinates, but it is expected to be constant in time. The default is set to 0 m.

MATERIAL

The default **Density** ρ (SI unit: kg/m^3) is taken **User defined**. Enter a different value or expression. The default is 1000 kg/m^3. The density can also be set **From material**. In that case, select the **Material** to use. By default, the material used is the **Domain material**. This corresponds to the material currently applied to the domain in question.

The value of the density is not used when solving but to compute the hydrostatic pressure and pressure force.

Domain Source

The **Domain Source** node specifies a momentum source on the right hand-side of the momentum equation

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \left(\mathbf{u} \otimes \mathbf{q} + g\frac{h}{2}\mathbf{I} \right) = -gh_B \nabla h_B + \mathbf{F}$$

This source term can model different effects, such as bottom friction, the Coriolis force, or wind stresses.

Initial Values

The **Initial Values** node adds an initial value for the water depth and water flux that serve as an initial condition for a transient simulation. If more than one set of initial values is required, add additional **Initial Values** nodes from the **Physics** toolbar.

INITIAL VALUES

Select the set of variables to be defined in **Initial values** — **Primitive variables** (the default), or **Conservative variables**.

For the **Water depth**, select **Specify water depth** (the default) or **Specify total height**.

- For **Specify water depth** provide a value or an expression for the water depth. The default is 0 m.
- For **Specify total height** provide a value or an expression for the **Total height** of the water column H. The default is 0 m. When using this option, the initial water depth is calculated as

$$h = \max(0, H - h_b)$$

The variable used to define the water flux $\mathbf{q}$ will depend on the selection of the **Initial values** selection list:

- For **Primitive variables** provide a value or an expression for the components of the velocity $\mathbf{u}$. The default is 0 m /s. The initial water depth is then calculated as

$$\mathbf{q} = h\mathbf{u}$$

- For **Conservative variables** provide a value or an expression for the components of the water flux $\mathbf{q}$. The default is 0 m^2 /s.

Inlet

Use the **Inlet** node to define boundaries where the fluid enters the domain. This condition uses the HLLC Riemann Solver (Ref. 1) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW PROPERTIES

Select the set of variables to be defined in **Input State** — **Primitive variables** (the default), or **Conservative variables**.

For the **Water depth**, select **User defined** (the default), **From domain values**, or **Specify total height**.

- For **User defined** provide a value or an expression for the water depth h_0. The default is 0 m.
- When **From domain values** is selected, the value of the water depth used to define the external state is taken from the solution at the boundary. Note that at supercritical inlets both water depth and water flux should be specified.
- For **Specify total height** provide a value or an expression for the **Total height** of the water column H_0. The default is 0 m. When using this option, the external water depth is calculated as

$$h_0 = \max(0, H_0 - h_b)$$

The variable used to define the water flux $\mathbf{q}_0$ will depend on the **Input state**:

- For **Primitive variables** the velocity is provided. If **User defined** is select, provide a value or an expression for the components of the velocity $\mathbf{u}_0$. The default is 0 m /s. The incoming water flux is then calculated as

$$\mathbf{q}_0 = h_0 \mathbf{u}_0$$

If **From domain values** is selected, the value of the velocity used to define the external state is taken from the solution at the boundary. Note that at supercritical inlets both water depth and water flux should be specified.

- For **Conservative variables** the water flux is required. If **User defined** is select, provide a value or an expression for the components of the water flux $\mathbf{q}_0$. The default value is 0 m^2 /s. If **From domain values** is selected, the value of the water flux used to define the external state is taken from the solution at the boundary. Note that at supercritical inlets both water depth and water flux should be specified.

Outlet

The **Outlet** node defines boundaries where the fluid leaves the domain. This condition uses the HLLC Riemann Solver (Ref. 1) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW PROPERTIES

Select the set of variables to be defined in **Input State** — **Primitive variables** (the default), or **Conservative variables**.

For the **Water depth**, select **User defined** (the default), **From domain values**, or **Specify total height**.

- For **User defined** provide a value or an expression for the water depth h_0. The default is 0 m.
- When **From domain values** is selected, the value of the water depth used to define the external state is taken from the solution at the boundary. Note that in supercritical outlets both water depth and water flux should be taken from domain values.
- For **Specify total height** provide a value or an expression for the **Total height** of the water column H_0. The default is 0 m. When using this option, the external water depth is calculated as

$$h_0 = \max(0, H_0 - h_b)$$

The variable used to define the external water flux $\mathbf{q}_0$ will depend on the **Input state**:

- For **Primitive variables** the velocity is provided. If **User defined** is select, provide a value or an expression for the components of the velocity $\mathbf{u}_0$. The default is 0 m /s. The outgoing water flux is then calculated as

$$\mathbf{q}_0 = h_0\mathbf{u}_0$$

If **From domain values** is selected, the value of the velocity used to define the external state is taken from the solution at the boundary. Note that in supercritical outlets both water depth and water flux should be taken from domain values.

- For **Conservative variables** the water flux is required. If **User defined** is select, provide a value or an expression for the components of the water flux $\mathbf{q}_0$. The default value is 0 m^2 /s. If **From domain values** is selected, the value of the water flux used to define the external state is taken from the solution at the boundary. In supercritical outlets both water depth and water flux should be taken from domain values.

Wall

The **Wall** node includes a set of boundary conditions preventing fluid flow in the direction perpendicular to the boundary. A no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, is enforced. Since viscous effects are neglected, no boundary layer develops.

The no-penetration condition is imposed weakly setting the following flux:

$$\Gamma_h \cdot \mathbf{n} = 0$$

$$-\Gamma_q \cdot \mathbf{n} = g\frac{h^2}{2}\mathbf{n}$$

- Theory for the Shallow Water Equations Interface

Symmetry

The **Symmetry** boundary condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. This node sets the same flux condition as the Wall feature.

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at $r = 0$. The software automatically provides an **Axial Symmetry** node prescribing $\mathbf{u} \cdot \mathbf{n} = 0$ on the axial symmetry boundaries.

Interior Wall

The **Interior Wall** node prevents fluid flow in the direction perpendicular to the boundary. It can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall condition can be used to avoid meshing thin structures by applying a no-penetration condition on interior curves and surfaces instead.

Water Source

The **Water Source** node specifies a height source in the continuity equation

$$\frac{\partial h}{\partial t} + \nabla \cdot \mathbf{q} = Q$$

Theory for the Shallow Water Equations Interface

This section describes the theory for the Shallow Water Equations, Time Explicit interface:

- The Shallow Water Equations
- The Numerical Method
- Wave Speed and Flow Regimes
- Forces on Boundaries
- References for the Shallow Water Equations Interfaces

The Shallow Water Equations

Figure 10-2 shows a typical configuration for the flow of fluid in a shallow layer. The upper boundary is referred to as the free surface and the lower boundary of the water layer is referred to as the bottom. The bottom height, h_b, is measured with respect to a reference xy-plane placed at $z = 0$ and it is assumed to be constant in time. The total height of the free surface is denoted H. The height of the water layer is typically measured in relation to the bottom height and denoted h. In dry regions, $h = 0$ and $H = h_b$.

The equations of continuity and momentum of incompressible inviscid flow subjected to gravity in the vertical direction ($\mathbf{g} = [0, 0, -g]^T$) are

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{10-1}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x} \tag{10-2}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y} \tag{10-3}$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} - g \tag{10-4}$$

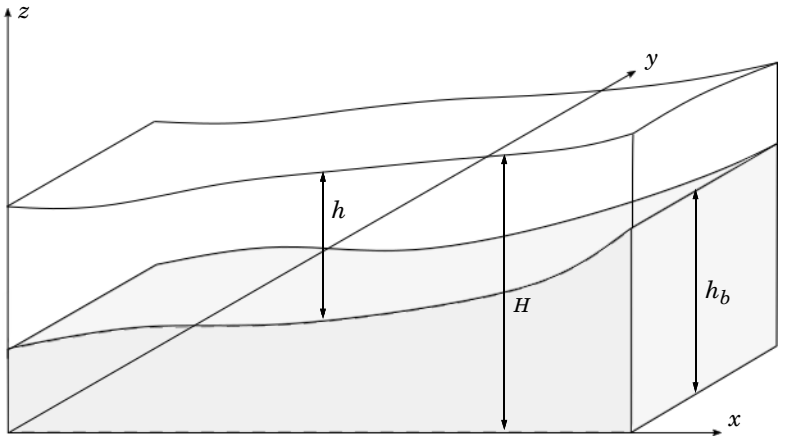

Figure 10-2: An example illustrating a typical configuration for shallow water equations. A water layer of thickness h flows over a nonflat bottom with topography represented by h_b. The total height of the free surface over the reference xy plane at $z = 0$ is represented by H. The gravity points downward (–z direction) and gives rise to a hydrostatic pressure ranging from 0 atm *at the free surface to a value of* $p = \rho \mathbf{g} h$ *at the bottom.*

Assuming that the water depth h is much smaller than the lateral dimensions of the geometry, the vertical accelerations can be neglected, $\frac{Dw}{Dt} = 0$, and Equation 10-4 reduces to the hydrostatic pressure relation

$$\frac{\partial p}{\partial z} = -\rho g \Rightarrow p = \rho g(h + h_b - z) \tag{10-5}$$

Both $h(x, y)$ and $h_b(x, y)$ are independent of z, implying that $\frac{\partial p}{\partial x} = \frac{\partial p}{\partial y} = 0$. Equation 10-2 and Equation 10-3 then reduces to

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -g\frac{\partial}{\partial x}(h + h_b) \tag{10-6}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -g\frac{\partial}{\partial y}(h + h_b) \tag{10-7}$$

which is the momentum equation of the 2D shallow water equations in nonconservative form. Note that u and v represent the horizontal velocity components averaged over h.

The continuity equation is recovered from Equation 10-1 when assuming no penetration on both the free surface and bottom boundaries:

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} uh + \frac{\partial}{\partial y} vh = 0 \tag{10-8}$$

See Chapter 2 in Ref. 1 for more details. Equation 10-6, Equation 10-7, and Equation 10-8 can be combined to express the shallow water equations in conservative form

$$\frac{\partial h}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0$$

$$\frac{\partial q_x}{\partial t} + \frac{\partial}{\partial x}\left(uq_x + g\frac{h^2}{2}\right) + \frac{\partial}{\partial y}(uq_y) = -gh\frac{\partial h_b}{\partial x} \tag{10-9}$$

$$\frac{\partial q_y}{\partial t} + \frac{\partial}{\partial x}(vq_x) + \frac{\partial}{\partial y}\left(vq_x + g\frac{h^2}{2}\right) = -gh\frac{\partial h_b}{\partial y} \tag{10-10}$$

q_x and q_y are the components of the water flux in the x and y directions, respectively. The vector $\mathbf{q} = [q_x, q_y, 0]^T$ can be obtained from the horizontally averaged velocity $\mathbf{u} = [u, v, 0]^T$ as

$$\mathbf{q} = \mathbf{u}h \tag{10-11}$$

Two different sets of variables are used in the context of the shallow water equations: the conservative variables h and $\mathbf{q}$, and the primitive variables h and $\mathbf{u}$.

The Numerical Method

The physics interface solves the shallow water equations using the Discontinuous Galerkin (DG) method in space together with explicit time stepping. The computations are restricted to transient problems. The basis functions are the nodal discontinuous Lagrange shape functions with constant order.

The numerical method used solves wave problems of the form

$$\mathbf{d}_\mathbf{a}\frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \Gamma(\mathbf{w}) = \mathbf{f}$$

When solving the shallow water equations, $\mathbf{d}_a$ is an identity matrix, $\mathbf{w}$ is the vector of conservative variables, Γ represents the conservative fluxes, and $\mathbf{f}$ includes the source terms:

$$\mathbf{w} = \begin{bmatrix} h \\ \mathbf{q} \end{bmatrix}$$

$$\Gamma(\mathbf{w}) = \begin{bmatrix} \Gamma_h \\ \Gamma_q \end{bmatrix} = \begin{bmatrix} \mathbf{q}^T \\ \mathbf{q} \otimes \mathbf{u} + g\frac{h^2}{2}\mathbf{I} \end{bmatrix}$$

$$\mathbf{f} = \begin{bmatrix} 0 \\ -gh\nabla h_b \end{bmatrix}$$

Here, Γ_h and Γ_q represent the fluxes of the continuity and momentum equations, respectively.

Discontinuous Galerkin methods use shape functions that are continuous in the interior of each mesh element, but discontinuous across element boundaries. A numerical flux must be defined between element boundaries and the dependent variables are not required to be continuous on faces between adjacent mesh elements. The default numerical flux is the **Lax-Friedrichs** flux, which uses an average of the physical fluxes together with a penalty term.

After discretization in space, the system of equations is integrated in time. The standard procedure is to use an explicit **Runge-Kutta** method. The physics interface uses the third-order SSP (strong stability preserving) Runge–Kutta method per default.

The time step in explicit computations is limited by the CFL condition; see Time Explicit Integrator in the *COMSOL Multiphysics Reference Manual*. The maximum stable time step is proportional to the smallest mesh element size h and inversely proportional to the maximum wave speed in the domain. On unstructured meshes with local refinement regions only a few elements are small, yet these dictate the overall time step for the whole problem. In such cases, the use of Local Time Stepping is

advisable. COMSOL Multiphysics provides the **Adams-Bashforth 3 (local)** time stepping method.

Theory for the Wave Form PDE in the *COMSOL Multiphysics Reference Manual*.

The bottom topography h_b is entered as a user-defined expression. In order to ensure that its gradient can be evaluated and is constant on every element, it is first projected onto the variable `swe.hb_linear` using linear Lagrangian shape functions. For plotting purposes, the provided expression for h_b is also projected onto the variable `swe.hb_constant` using the same piecewise discontinuous shape functions as for h. These projections are done in a Stationary study step that must be computed before the Time Dependent study step is used to compute the shallow water equations. When starting a new model from the **Model Wizard**, the stationary study step is added per default when selecting a Time Dependent study.

Wave Speed and Flow Regimes

The fluxes of the momentum and continuity equations, $\Gamma(\mathbf{w})$, provide information about the speed of the waves. The eigenvalues of the Jacobian matrix of the fluxes evaluated at a direction provided by an arbitrary unit vector $\mathbf{n} = [n_x, n_y, 0]^T$ are

$$\lambda_1 = \mathbf{u} \cdot \mathbf{n} - c, \lambda_2 = \mathbf{u} \cdot \mathbf{n}, \lambda_3 = \mathbf{u} \cdot \mathbf{n} + c$$

where c is the wave celerity,

$$c = \sqrt{gh}$$

The eigenvalues of the Jacobian of the fluxes provide information about the velocity at which information is propagated. When $|\mathbf{u} \cdot \mathbf{n}| > c$, the eigenvalues have different sign and information is propagated both upward and downward. If $|\mathbf{u} \cdot \mathbf{n}| < c$, all eigenvalues have the same sign and all waves travel in the same direction.

The Froude number Fr is a dimensionless number typically used to define the flow regime by specifying the ratio of the inertial forces to gravity forces. In case of the Shallow Water Equations, it is defined as

$$\mathrm{Fr} = \frac{|\mathbf{u}|}{c}$$

The flow regime can be divided into subcritical flow, $\mathbf{Fr} < 1$, and supercritical flow, $\mathbf{Fr} > 1$. This classification is specially important when defining boundary conditions. In supercritical flows, all characteristics must be specified at inlets and extrapolated from the domain at outlets. In subcritical flows, the characteristics are partially specified from exterior values and partially extrapolated from interior values for both inlets and outlets.

Forces on Boundaries

The physics interface provides variables to compute the pressure force acting on boundaries. In the shallow water equations the pressure is assumed to be hydrostatic

$$p = \rho g(h + h_b - z)$$

The pressure force per unit length on a boundary can be obtained integrating along h

$$\mathbf{F}_p = \int_h^0 \rho g z \mathbf{n} dz = \rho g \frac{h^2}{2} \mathbf{n}$$

The components of the vector $\mathbf{F_p}$ are available as variables in the Shallow Water Equations, Time Explicit physics interface and can be accessed in 2D using `swe.Fpx` and `swe.Fpy`. In 1D only the `swe.Fpx` component is defined. Note that these variables represent a force per unit length; the total force on a boundary is obtained integrating over the whole boundary.

The *Dam Breaking on a Column, Shallow Water Equations* Application Library model is an example of how to use these variables. Application Library path **CFD_Module/Shallow_Water_Equations/dam_break_column_sw**

References for the Shallow Water Equations Interfaces

1. E.F. Toro, *Shock capturing methods for free-surface shallow flows*, John Wiley & Sons, 2001.

11

Mathematics, Moving Interface Branch

The Level Set and Phase Field in Fluids Moving interfaces are available under the **Mathematics** > **Moving Interface** branch ( ). Also see Modeling Multiphase Flow to help you choose the best interface to start with.

In this chapter:

- The Level Set Interface
- The Phase Field in Fluids Interface
- The Phase Field Thin-Film Flow Interfaces
- The Ternary Phase Field Interface
- Theory for the Level Set Interface
- Theory for the Phase Field in Fluids Interface
- Theory for the Phase Field Thin-Film Flow Interfaces
- Theory for the Ternary Phase Field Interface

The Level Set Interface

In this section:

- The Level Set Interface
- The Level Set in Porous Media Interface
- Domain, Boundary, and Pair Nodes for the Level Set Interface

The Level Set Interface

The **Level Set (ls)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding an interface, is used to track moving interfaces in fluid-flow models by solving a transport equation for the level set function. Simulations using the **Level Set** interface are always time dependent because the position of an interface almost always depends on its history.

The main node is the Level Set Model feature, which adds the level set equation and provides an interface for defining the level set properties and the velocity field.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Level Set Model**, **No Flow** (the default boundary condition), **Initial Values**, and **Initial Values, Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Level Set** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `ls`.

STABILIZATION

To display this sections, click the **Show More Options** button ( ) and select **Stabilization** in the **Show More Options** dialog.

There are two stabilization methods available — **Streamline diffusion** and **Crosswind diffusion**. Both are active by default and should remain selected for optimal performance.

ADVANCED SETTINGS

To display this sections, click the **Show More Options** button ( ) and select **Advanced Physics Options** in the **Show More Options** dialog.

Specify the **Convective term** as **Nonconservative form** (default) or **Conservative form**.

DISCRETIZATION

By default, the Level Set interface uses **Linear** elements. When coupling the physics interface to a fluid flow interface by means of The Two-Phase Flow, Level Set Coupling Feature, exact conservation of the integral of ϕ is obtained using the nonconservative form provided that the discretization order of the level set variable is equal to or lower than the order of the pressure.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Level set variable** phi. The name can be changed but the names of fields and dependent variables must be unique within a model.

- Conservative and Nonconservative Form
- Domain, Boundary, and Pair Nodes for the Level Set Interface
- Theory for the Level Set Interface
- Theory for the Two-Phase Flow Interfaces

The Level Set in Porous Media Interface

The **Level Set in Porous Media (ls)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding an interface, is used to track moving interfaces in fluid-flow through porous media models by solving a transport equation for the level set function. Simulations using the **Level Set in Porous Media** interface are always time dependent since the position of an interface almost always depends on its history.

The main node is the Porous Medium Level Set Model feature, which adds the level set equation and provides interfaces for defining the level set properties, the velocity field and the porosity of the porous matrix.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Porous Medium**, **No Flow** (the default boundary condition), **Initial Values**, and **Initial Values, Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Level Set in Porous Media** to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as for the **Level Set** interface.

Domain, Boundary, and Pair Nodes for the Level Set Interface

The Level Set Interface has the following domain, boundary, and pair nodes described.

- Continuity
- Initial Values
- Inlet
- Level Set Model
- No Flow
- Open Boundary
- Outlet[1]
- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Porous Matrix
- Porous Medium
- Symmetry[1]
- Thin Barrier

[1] Described for the Laminar Flow interface.

Boundary conditions for axial symmetry boundaries are not required. For the symmetry axis at $r = 0$, the software automatically provides a suitable boundary condition and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Level Set Model

If the **Level Set Model** node is a domain feature under The Level Set Interface, it adds the following transport equation governing a level set function ϕ:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$

If it is a domain subfeature under the Porous Medium domain feature, it adds the following equation:

$$\varepsilon_p \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$

In both cases, the **Level Set Model** node provides the options to define the associated level set parameters and the velocity field.

LEVEL SET PARAMETERS

Enter a value or expression for the **Reinitialization parameter** γ (SI unit: m/s). The default is 1 m/s.

Enter a value or expression for the **Parameter controlling interface thickness** ε_{ls} (SI unit: m). The default expression is `ls.ep_default`, a value proportional to the maximum element size with a proportionality factor dependent on the ratio of the maximum and minimum element sizes in the domain.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** $\mathbf{u}$ (SI unit: m/s). The applied velocity field transports the level set function through convection.

Porous Medium

The **Porous Medium** node adds the level set equation. It has two default subfeatures — the Level Set Model feature where the reinitialization parameter γ (SI unit: m/s) and the parameter controlling the interface thickness ε_{ls} (SI unit: m) are defined, and the Porous Matrix feature where the porosity ε_p (dimensionless) is specified.

Porous Matrix

This node contains inputs for the material properties of the solid matrix of the Porous Medium parent node.

MATRIX PROPERTIES

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material**. For **User defined** the default is 1.

Initial Values

Use the **Initial Values** node to define the initial values of the level set variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the separating interface, can be specified in two ways. The level set function can be specified explicitly using any type of variable or expression. Alternatively, the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the level set function across the fluid-fluid interface.

Specify the **Level set variable** as one of the following:

- To specify the fluid occupying the domain, select **Specify phase** (default). Then select the checkbox **Fluid 1 ($\phi = 0$)** or **Fluid 2 ($\phi = 1$)**.
- For **User defined** enter a value or expression for the level set variable ϕ.

If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid 1 ($\phi = 0$)** and the other **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

See Initializing the Level Set Function.

Inlet

LEVEL SET CONDITION

Specify **Level Set Condition** according to one of the following options:

- **Fluid 1 ($\phi = 0$)**
- **Fluid 2 ($\phi = 1$)**
- **Specify level set function explicitly**

When the **Specify level set function explicitly** is selected, the level set function ϕ must be specified explicitly. The value must be in the range from 0 to 1, where the default is 0.

No Flow

The **No Flow** node adds a boundary condition that represents boundaries where there is no flow across the boundary. This is the default boundary condition.

Open Boundary

Use this node to set up transport across boundaries where both convective inflow and outflow can occur. On the parts of the boundary where fluid flows into the domain, an exterior value of the level set function is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Level Set interface.

LEVEL SET CONDITION

Specify **Level Set Condition** according to one of the following options:

- **Fluid 1 ($\phi = 0$)**
- **Fluid 2 ($\phi = 1$)**
- **Specify level set function explicitly**

When the **Specify level set function explicitly** is selected, the level set function ϕ must be specified explicitly. The value must be in the range from 0 to 1, where the default is 0.

Thin Barrier

The **Thin Barrier** feature is available on interior boundaries and introduces a discontinuity in the level set variable across the boundary. A No Flow condition is prescribed on each side. This node can be used to avoid meshing thin structures.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the level set variable is continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts. By default, the No Flow node is used as fallback unless another feature has been selected for the boundary.

About Pairs

LOCATION IN USER INTERFACE

Right-click the physics interface and select **Pairs** > **Continuity**.

Ribbon

Physics tab with the physics interface selected:

Pairs > **Continuity**

The Phase Field in Fluids Interface

The **Phase Field in Fluids (pf)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding a physics interface, is used to track moving fluid-fluid interfaces by solving two transport equations, one for the phase field variable, ϕ, and one for the mixing energy density, ψ. The position of the interface is determined by minimizing the free energy.

The main node is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Phase Field Model**, **Wetted Wall** (the default boundary condition), **Initial Values**, and **Initial Values, Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Phase Field in Fluids** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `pf`.

ADVANCED SETTINGS

To display this sections, click the **Show More Options** button ( ) and select **Advanced settings options** in the **Show More Options** dialog.

Specify the **Convective term** as **Nonconservative form** (default) or **Conservative form**.

DISCRETIZATION

By default, the Phase Field in Fluids interface uses **Linear** elements.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields) **Phase field variable** ϕ and **Phase field help variable** ψ. If required, edit the name, but dependent variables must be unique within a model.

- Conservative and Nonconservative Forms
- Domain, Boundary, and Pair Nodes for the Phase Field in Fluids Interface
- Theory for the Phase Field in Fluids Interface

Phase Separation: Application Library path
CFD_Module/Multiphase_Flow/phase_separation

Domain, Boundary, and Pair Nodes for the Phase Field in Fluids Interface

The Phase Field in Fluids Interface includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Continuity
- Initial Values
- Inlet
- Interior Wetted Wall
- Outlet
- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Phase Field Model
- Symmetry
- Wetted Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Phase Field Model

The **Phase Field Model** node adds the equations described in The Equations for the Phase Field Method. The node defines the associated phase field parameters including surface tension and interface thickness.

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- **Surface tension coefficient** σ (SI unit: N/m).
- **Parameter controlling interface thickness** ε_{pf} (SI unit: m). The default expression is `pf.ep_default`, a value proportional to the maximum element size with a proportionality factor dependent on the ratio of the maximum and minimum element sizes in the domain.
- **Mobility tuning parameter** χ (SI unit: m·s/kg). This parameter determines the time scale of the Cahn–Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Select **User defined** (default) or **Calculate from velocity**. For **User defined** enter a value or expression for the mobility tuning parameter χ. The default is 1 m·s/kg, which is a good starting point for most models.

  For **Calculate from velocity** enter a value for the expected velocity at the interface U (SI unit: m/s). χ is then computed as:

$$\chi = \frac{Uh_{\max}}{3\sqrt{2}\sigma\varepsilon}$$

  where $h_{\max}$ is the largest mesh cell size.

Keep the χ parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets.

EXTERNAL FREE ENERGY

Add a source of external free energy to the phase field equations. This modifies the last term on the right-hand side of the equation:

$$\psi = -\nabla \cdot \varepsilon^2 \nabla\phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial \phi}$$

The external free energy f (SI unit: $\mathrm{J/m^3}$) is a user-defined free energy. In most cases, the external free energy can be set to zero. Manually differentiate the expression for the external free energy with respect to ϕ and then enter it into the **ϕ-derivative of external free energy** field $\partial f/\partial\phi$.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** u (SI unit: m/s). The applied velocity field transports the phase field variables through convection.

Additional Sources of Free Energy

Initial Values

Use the **Initial Values** node to define the initial values of the phase field variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the fluid-fluid interface, can be specified in two ways. The phase field variable can be specified explicitly, using any type of variable or expression. Alternatively the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the phase field function across the fluid-fluid interface.

Specify the **Phase field variable** as one of the following:

- To specify the fluid occupying the domain, select **Specify phase** (default). Then select the checkbox **Fluid 1** ($\phi = -1$) or **Fluid 2** ($\phi = 1$).
- For **User defined** enter a value or expression for the phase field variable ϕ.

!	If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes is set to **Specify phase: Fluid 1 ($\phi = -1$)** and the other to **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

Inlet

SETTINGS

Specify **Phase field Condition** according to one of the following options:

- **Fluid 1 ($\phi = -1$)**
- **Fluid 2 ($\phi = 1$)**
- **Specify phase field function explicitly**

When **Specify phase field function explicitly** is selected, the phase field function ϕ must be specified in the entire domain. The value must be in the range from -1 to 1, where the default is 1.

Wetted Wall

The **Wetted Wall** node is the default boundary condition representing wetted walls. Along a wetted wall the contact angle for the fluid, θ_w, is specified, and across it, the mass flow is zero. This is prescribed by

$$\mathbf{n} \cdot \varepsilon^2 \nabla\phi = \varepsilon^2 \cos(\theta_w)|\nabla\phi|$$

in combination with

$$\mathbf{n} \cdot \frac{\gamma\lambda}{\varepsilon^2}\nabla\psi = 0$$

The contact angle θ_w can be defined directly or from Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_w) + \gamma_{s2} = \gamma_{s1} \tag{11-1}$$

where γ_{s1} is the surface energy density on the fluid 1 — solid (wall) interface and γ_{s2} is the surface energy density on the fluid 2 — solid (wall) interface.

WETTED WALL

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**. For **Directly** enter a value or expression for the **Contact angle** θ_w (SI unit: rad). The default value is $\pi/2$ radians. For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

Interior Wetted Wall

The **Interior Wetted Wall** feature is available on interior boundaries. It is similar to the Wetted Wall condition except that it applies on both sides of an interior boundary and introduces a discontinuity of the phase field variables across the boundary. This node can be used to avoid meshing thin structures.

Along an interior wetted wall the contact angle for the fluid, θ_w, is specified on both sides of the boundary, and across it, the mass flow is zero.

WETTED WALL

Enter a value or expression for the **Contact angle** θ_w. The default value is $\pi/2$ rad.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the phase field variables are continuous across the pair.

The parts of the boundary where a source boundary lacks a corresponding destination boundary and vice versa will get conditions from other boundary conditions under the physics interface acting as fallback boundary conditions on the nonoverlapping parts.

By default, the Wetted Wall node is used as fallback unless another feature has been selected for the boundary.

About Pairs

LOCATION IN USER INTERFACE

Right-click the physics interface and select **Pairs** > **Continuity**.

Ribbon

Physics tab with the physics interface selected:

Pairs > **Continuity**

The Phase Field Thin-Film Flow Interfaces

The **Phase Field Thin-Film Flow (pftff)** interface for 2D problems ( ) and **Phase Field Thin-Film Flow (pftff)** interface for 3D problems ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding a physics interface, are used to track moving interfaces by solving two transport equations, one for the phase field variable, ϕ, and one for the mixing energy density, ψ, in thin-film flows. The fluids are assumed to flow in a narrow channel, that is represented, within the geometry, by an edge for 2D problems and a surface for 3D in the **Phase Field Thin-Film Flow (pftff)** interface. The position of the interface is determined by minimizing the free energy.

The main node is the Phase Field Model feature, which adds the phase field thin-film flow equations and provides an interface for defining the phase field model properties.

When the **Phase Field Thin-Film Flow (pftff)** interface for 2D is added, the following default nodes are also added in the **Model Builder** — **Phase Field Model**, **Initial Values**, and **Initial Values, Fluid 2**. And when the **Phase Field Thin-Film Flow (pftff)** physics interface for 3D problems is added, the following default nodes are also added in the **Model Builder** — **Phase Field Model**, **Wetted Wall** (the default boundary condition), **Initial Values**, and **Initial Values, Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Phase Field Thin-Film Flow (pftff)** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern *<name>*.*<variable_name>*. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `pftff`.

ADVANCED SETTINGS

To display this sections, click the **Show More Options** button ( ) and select **Advanced settings options** in the **Show More Options** dialog.

Specify the **Convective term** as **Nonconservative form** (default) or **Conservative form**.

DISCRETIZATION

By default, the Phase Field Thin-Film Flow interface uses **Linear** elements.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields) **Phase field variable** ϕ and **Phase field help variable** ψ. If required, edit the name, but dependent variables must be unique within a model.

- Conservative and Nonconservative Forms
- Boundary, Edge, and Point Nodes for the Phase Field Thin-Film Flow Interfaces
- Theory for the Phase Field Thin-Film Flow Interfaces

Boundary, Edge, and Point Nodes for the Phase Field Thin-Film Flow Interfaces

The Phase Field Thin-Film Flow Interfaces include the following boundary, edge, and point nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Initial Values
- Inlet
- Interior Wetted Wall
- Outlet
- Phase Field Model
- Symmetry
- Wetted Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Phase Field Model

The Equations for the Phase Field Thin-Film Flow Method are added in the **Phase Field Model** node. The node defines the associated phase field parameters including surface tension and interface thickness.

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- **Surface tension coefficient** σ (SI unit: N/m).
- **Parameter controlling interface thickness** ε_{pf} (SI unit: m). The default expression is `pftff.ep_default`, a value proportional to the maximum element size with a proportionality factor dependent on the ratio of the maximum and minimum element sizes in the domain.
- **Mobility tuning parameter** χ (SI unit: m·s/kg). This parameter determines the time scale of the Cahn–Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Select **User defined** (default) or **Calculate from velocity**. For **User defined** enter a value or expression for the mobility tuning parameter χ. The default is 1 m·s/kg, which is a good starting point for most models.

  For **Calculate from velocity** enter a value for the expected velocity at the interface U (SI unit: m/s). χ is then computed as:

$$\chi = \frac{Uh_{\max}}{3\sqrt{2}\sigma\varepsilon}$$

  where $h_{\max}$ is the largest mesh cell size.

Keep the χ parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets.

EXTERNAL FREE ENERGY

Add a source of external free energy to the phase field equations. This modifies the last term on the right-hand side of the equation:

$$\psi = -\nabla_t \cdot \varepsilon^2 \nabla_t \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial \phi}$$

The external free energy f (SI unit: J/m^3) is a user-defined free energy. In most cases, the external free energy can be set to zero. Manually differentiate the expression for the external free energy with respect to ϕ and then enter it into the **ϕ-derivative of external free energy** field $\partial f/\partial\phi$.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** u (SI unit: m/s). The applied velocity field transports the phase field variables through convection.

Additional Sources of Free Energy

Wetted Wall

The **Wetted Wall** node is the default boundary condition representing wetted walls. Along a wetted wall the contact angle for the fluid, θ_w, is specified, and across it, the mass flow is zero. This is prescribed by

$$\mathbf{n} \cdot \varepsilon^2 \nabla_t \phi = \varepsilon^2 \cos(\theta_w)\left|\nabla_t \phi\right|$$

in combination with

$$\mathbf{n} \cdot \frac{\gamma\lambda}{\varepsilon^2}\nabla_t \psi = 0$$

The contact angle θ_w can be defined directly or from Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_w) + \gamma_{s2} = \gamma_{s1} \tag{11-2}$$

where γ_{s1} is the surface energy density on the fluid 1 — solid (wall) interface and γ_{s2} is the surface energy density on the fluid 2 — solid (wall) interface.

WETTED WALL

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**. For **Directly** enter a value or expression for the **Contact angle** θ_w (SI unit: rad). The default value is $\pi/2$ radians. For **Through Young's equation** enter values or expressions for **Phase 1-Solid surface energy density** γ_{s1} (SI unit: J/m^2) and **Phase 2-Solid surface energy density** γ_{s2} (SI unit: J/m^2).

The wetted wall condition is not available for the **Phase Field Thin-Film Flow (pftff)** interface for 2D problems.

Interior Wetted Wall

The **Interior Wetted Wall** feature is available on interior boundaries. It is similar to the Wetted Wall condition except that it applies on both sides of an interior boundary and introduces a discontinuity of the phase field variables across the boundary. This node can be used to avoid meshing thin structures.

Along an interior wetted wall the contact angle for the fluid, θ_w, is specified on both sides of the boundary, and across it, the mass flow is zero.

WETTED WALL

Enter a value or expression for the **Contact angle** θ_w. The default value is $\pi/2$ rad.

The interior wetted wall condition is not available for the **Phase Field Thin-Film Flow (pftff)** interface for 2D problems.

The Ternary Phase Field Interface

The **Ternary Phase Field (terpf)** interface ( ), found under the **Mathematics** > **Moving Interface** branch ( ) when adding a physics interface, is used to track moving interfaces separating three different phases. The interface solves four transport equations: two equations governing phase field variables, ϕ_A and ϕ_B, and two equations for the corresponding generalized chemical potentials, η_A and η_B. The position of the interfaces are determined by minimization of the free energy.

The phase field variables are defined such that they represent the volume fraction of the respective phase. The volume fraction of the third phase not solved for, but computed from the natural constraint that the sum of the volume fractions of all phases is one.

The main node of the interface is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties such as surface tensions and parameters controlling the interface thickness.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Mixture Properties**, **Wetted Wall** and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Ternary Phase Field** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `terpf`.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields):

- **Phase field variable, fluid A** `phiA`
- **Phase field variable, fluid B** `phiB`

- **Generalized chemical potential of fluid A** `etaA`
- **Generalized chemical potential of fluid B** `etaB`

If required, edit the any of the names, but dependent variables must be unique within a model.

Theory for the Phase Field Thin-Film Flow Interfaces

Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface

The Phase Field Thin-Film Flow Interfaces includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking the interface node to access the context menu (all users).

- Initial Values
- Inlet
- Outlet
- Phase Field Model
- Symmetry
- Wetted Wall

Mixture Properties

The **Mixture Properties** node adds the equations described in The Equations of the Ternary Phase Field Method. The node defines the associated phase field parameters, including the surface tension coefficients and parameters controlling the thickness of the interfaces.

MODEL INPUTS

The surface tension coefficients can be defined through user inputs, variables, or by selecting a material. For the latter option, an additional input, the temperature, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component,

it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T

Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

Parameter controlling interface thickness ε. The default expression is `terpf.ep_default*sqrt(2)`, a value proportional to the maximum element size with a proportionality factor dependent on the ratio of the maximum and minimum element sizes in the domain.

- **Mobility tuning parameter** M_0. This parameter determines the time scale of the Cahn–Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Keep the mobility tuning parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets. By default, M_0 is set to $1{\cdot}10^{-4}$ m^3/s, which is a good starting point for most models.
- **Additional free bulk energy** Λ. When needed, add a user-defined expression for the additional bulk energy.

SURFACE TENSION

Specify the surface tension coefficients for the three types of interfaces present.

- To use a predefined expression, select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface.** Then select an option from the list that displays below (**Water/Air**, **Glycerol/Air**, and so forth).
- For **User defined**, enter a value or expression for the surface tension coefficient.

The predefined correlations are based on the data in Ref. 3, Ref. 4, and Ref. 5.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D, for example) of the **Velocity field** u. The applied velocity field transports the phase field variables through convection.

Initial Values

The **Initial Values** node adds initial values for the phase field variables that can serve as initial conditions for a transient simulation.

INITIAL VALUES

Enter initial values or expressions for **Phase field variable A** and the **Phase field variable B** corresponding to the mass fraction of the respective phase. The value must be in the range from 0 to 1.

Inlet

This condition should be used on boundaries for which there is a net convective flow of the phases into the adjacent domain.

INLET

Specify phase field variables, corresponding to the volume fractions, of phase A and phase B. The value must be in the range from 0 to 1. The volume fraction of phase C will be evaluated such that the sum of all mass fractions equals one.

Mathematically this boundary condition imposes

$$\phi_i = \phi_{i,0}\,,\ \mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Outlet

This condition should be used on boundaries for which there is a net convective outflow from the domain.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Symmetry

Use this condition on boundaries that represent a geometrical symmetry line across which the flow of the fluid phases is zero.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases $i = A$ and B.

Wetted Wall

Use this node to represent a solid wall along which the contact angles between the separating interfaces and the wall should be prescribed.

WETTED WALL

Enter values or expressions for the contact angles for the three interfaces types:

- The **Contact angle of interface from phase A to phase C** θ_α.
- The **Contact angle of interface from phase B to phase C** θ_β.
- The **Contact angle of interface from phase A to phase B** θ_γ.

The definition of the contact angles with respect to the wall are shown in the figure below.

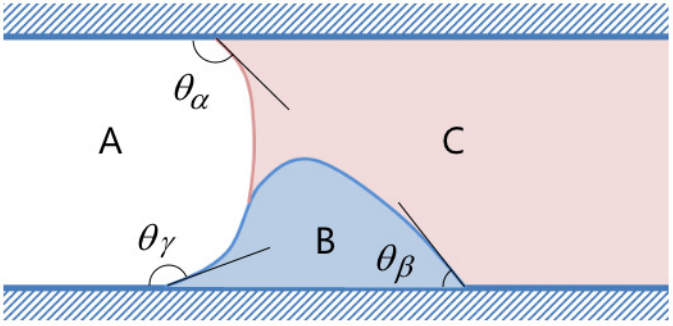

Figure 11-1: Definitions of the contact angels in the Wetted Wall feature of the Ternary Phase Field interface.

Theory for the Level Set Interface

Fluid flow with moving interfaces or boundaries occur in a number of different applications, such as *fluid-structure interaction*, multiphase flows, and flexible membranes moving in a liquid. One way to track moving interfaces is to use a level set method. A certain contour line of the globally defined function, the level set function, then represents the interface between the phases. For The Level Set Interface the fluid-fluid interface can be advected with an arbitrary velocity field.

In this section:

- The Level Set Method
- Conservative and Nonconservative Form
- Initializing the Level Set Function
- Variables For Geometric Properties of the Interface
- Reference for the Level Set Interface

The Level Set Method

The *level set method* is a technique to represent moving interfaces or boundaries using a fixed mesh. It is useful for problems where the computational domain can be divided into two domains separated by an interface. Each of the two domains can consist of several parts. Figure 11-2 shows an example where one of the domains consists of two separated parts. The interface is represented by a certain level set or isocontour of a globally defined function, the level set function ϕ. In COMSOL Multiphysics, ϕ is a smooth step function that equals zero (0) in one domain and one (1) in the other. Across the interface, there is a smooth transition from zero to one. The interface is

defined by the 0.5 isocontour, or level set, of ϕ. Figure 11-3 shows the level set representation of the interface in Figure 11-2.

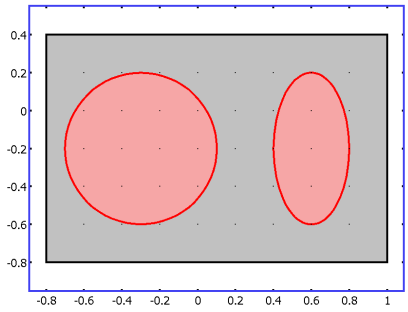

Figure 11-2: An example of two domains divided by an interface. In this case, one of the domains consists of two parts. Figure 11-3 *shows the corresponding level set representation.*

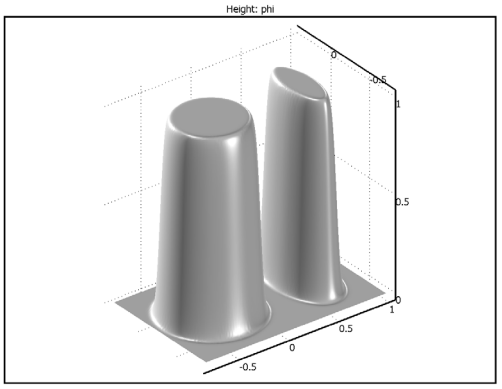

Figure 11-3: A surface plot of the level set function corresponding to Figure 11-2.

The physics interface solves Equation 11-3 in order to move the interface with the velocity field $\mathbf{u}$:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{11-3}$$

The terms on the left-hand side give the correct motion of the interface, while those on the right-hand side are necessary for numerical stability. The parameter, ε_{ls}, determines the thickness of the region where ϕ varies smoothly from zero to one and is typically of the same order as the size of the elements of the mesh. By default, ε_{ls} is

constant within each domain and proportional to the largest value of the mesh size, h, within the domain. The parameter γ determines the amount of reinitialization or stabilization of the level set function. It needs to be tuned for each specific problem. If γ is too small, the thickness of the interface might not remain constant and oscillations in ϕ can appear because of numerical instabilities. On the other hand, if γ is too large the interface moves incorrectly. A suitable value for γ is the maximum magnitude of the velocity field $\mathbf{u}$.

Conservative and Nonconservative Form

If the velocity is divergence free, that is, if

$$\nabla \cdot \mathbf{u} = 0 \tag{11-4}$$

the volume (area for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the boundaries. To obtain exact numerical conservation in cases where Equation 11-4 is not fully satisfied, switch to the conservative form

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{11-5}$$

in Settings window for The Level Set Interface.

Using the conservative level set form, exact numerical conservation of the integral of ϕ is obtained. However, the nonconservative form is better suited for numerical calculations and usually converges more easily. The nonconservative form, which is the default form, only conserves the integral of the level set function approximately, but this level of conservation is sufficient for most applications.

When the Level Set interface is coupled to a fluid-flow interface by means of The Two-Phase Flow, Level Set Coupling Feature, exact conservation of the integral of ϕ is obtained using the nonconservative form, provided that the discretization order of the level set variable is equal to or lower than the order of the pressure.

Rising Bubble: Application Library path
CFD_Module/Multiphase_Flow/rising_bubble_2daxi

The Level Set Equation in Porous Domains

In a porous domain, the equation that determines the evolution of the interface is

$$\frac{\partial \phi}{\partial t} + \mathbf{u}_{\text{pore}} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{\text{ls}} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{11-6}$$

Here $\mathbf{u}_{\text{pore}}$ is the pore velocity. Instead using the Darcy velocity $\mathbf{u}=\mathbf{u}_{\text{pore}}/\varepsilon_{\text{p}}$, multiplying the equation with the porosity ε_{p}, and rescaling γ such that it again can be set proportional to the maximum magnitude of the velocity field $\mathbf{u}$, the equation can be rewritten as:

$$\varepsilon_{\text{p}} \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{\text{ls}} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{11-7}$$

This is the nonconservative form of the level set equation that is solved in the Porous Medium feature.

To obtain exact numerical conservation of the integral of $\varepsilon_{\text{p}}\phi$, switch to the conservative form

$$\frac{\partial}{\partial t}(\varepsilon_{\text{p}} \phi) + \nabla \cdot (\mathbf{u}\phi) = \gamma \nabla \cdot \left(\varepsilon_{\text{ls}} \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{11-8}$$

The conservative form can be derived from the nonconservative form if it is assumed that the velocity field $\mathbf{u}$ satisfies the following continuity equation:

$$\frac{\partial \varepsilon_{\text{p}}}{\partial t} + \nabla \cdot \mathbf{u} = 0 \tag{11-9}$$

Initializing the Level Set Function

If the study type Transient with Phase Initialization is used in the model, the level set variable is first initialized so that it varies smoothly between zero and one over the interface. For that study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the level set function according to the following expression:

$$\phi_0 = \frac{1}{1 + e^{-D_{\text{wi}}/\varepsilon}}$$

in domains initially outside the interface and

$$\phi_0 = \frac{1}{1 + e^{D_{wi}/\varepsilon}}$$

in domains initially inside the interface. Here, inside refers to domains where $\phi < 0.5$ and outside refers to domains where $\phi > 0.5$.

If the **Transient with Phase Initialization** ( ) study is being used, then, for the initialization to work, it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid 1 ($\phi = 0$)** and the other **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

- The Level Set Interface
- Studies and Solvers and Time Dependent with Initialization in the *COMSOL Multiphysics Reference Manual*

Variables For Geometric Properties of the Interface

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi = 0{,}5} \tag{11-10}$$

This variable is available in the physics interface as the interface normal `ls.intnorm`.

Reference for the Level Set Interface

1. E. Olsson and G. Kreiss, "A Conservative Level Set Method for Two Phase Flow," *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

Theory for the Phase Field in Fluids Interface

The Phase Field in Fluids Interface theory is described in this section:

- About the Phase Field Method
- The Equations for the Phase Field Method
- Conservative and Nonconservative Forms
- Additional Sources of Free Energy
- Initializing the Phase Field Function
- Variables and Expressions
- Reference for the Phase Field in Fluids Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the interfacial layer is governed by a phase field variable, ϕ. The surface tension force is added to the Navier–Stokes equations as a body force by multiplying the chemical potential of the system by the gradient of the phase field variable.

The evolution of the phase field variable is governed by the *Cahn–Hilliard equation*, which is a 4th-order PDE. The Phase Field in Fluids interface decomposes the Cahn–Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn–Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of two immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple two-phase flows, only the mixing energy is retained, which results in a rather simple expression for the free energy.

The Equations for the Phase Field Method

The free energy is a functional of a dimensionless phase field parameter, ϕ:

$$F(\phi, \nabla\phi, T) = \int\left(\frac{1}{2}\varepsilon^2|\nabla\phi|^2 + f(\phi, T)\right)dV = \int f_{\text{tot}}dV$$

where ε is a measure of the interface thickness. Equation 11-11 describes the evolution of the phase field parameter:

$$\frac{\partial\phi}{\partial t} + (\mathbf{u}\cdot\nabla)\phi = \nabla\cdot\gamma\nabla\left(\frac{\partial f_{\text{tot}}}{\partial\phi} - \nabla\cdot\frac{\partial f_{\text{tot}}}{\partial\nabla\phi}\right) \tag{11-11}$$

where f_{tot} (SI unit: J/m^3) is the total free energy density of the system, and $\mathbf{u}$ (SI unit: m/s) is the velocity field for the advection. The right-hand side of Equation 11-11 aims to minimize the total free energy with a relaxation time controlled by the mobility γ (SI unit: $\text{m}^3\cdot\text{s/kg}$).

The free energy density of an isothermal mixture of two immiscible fluids is the sum of the mixing energy and elastic energy. The mixing energy assumes the Ginzburg–Landau form:

$$f_{\text{mix}}(\phi, \nabla\phi) = \frac{1}{2}\lambda|\nabla\phi|^2 + \frac{\lambda}{4\varepsilon^2}(\phi^2 - 1)^2$$

where ϕ is the dimensionless phase field variable, defined such that the volume fraction of the components of the fluid are $(1+\phi)/2$ and $(1-\phi)/2$. The quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon} \tag{11-12}$$

The PDE governing the phase field variable is the Cahn–Hilliard equation:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\gamma\nabla G \tag{11-13}$$

where G (SI unit: Pa) is the chemical potential and γ (SI unit: $\text{m}^3\cdot\text{s/kg}$) is the mobility. The mobility determines the time scale of the Cahn–Hilliard diffusion and must be large enough to retain a constant interfacial thickness but small enough so that the convective terms are not overly damped. In COMSOL Multiphysics the mobility is determined by a mobility tuning parameter that is a function of the interface thickness $\gamma = \chi\varepsilon^2$. The chemical potential is:

$$G = \lambda\left[-\nabla^2\phi + \frac{\phi(\phi^2 - 1)}{\varepsilon^2}\right] \tag{11-14}$$

The Cahn–Hilliard equation forces ϕ to take a value of 1 or –1 except in a very thin region on the fluid-fluid interface. The Phase Field in Fluids interface breaks Equation 11-13 up into two second-order PDEs:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi \tag{11-15}$$

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2 - 1)\phi \tag{11-16}$$

Conservative and Nonconservative Forms

If the velocity field is divergence free, that is, if

$$\nabla\cdot\mathbf{u} = 0 \tag{11-17}$$

the volume (area for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the boundaries. To obtain exact numerical conservation in cases where Equation 11-17 is not fully satisfied, switch to the conservative form

$$\frac{\partial\phi}{\partial t} + \nabla\cdot\mathbf{u}\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi$$

Using the conservative phase field form, exact numerical conservation of the integral of ϕ is obtained. However, the nonconservative form is better suited for numerical calculations and usually converges more easily. The nonconservative form, which is the default form, only conserves the integral of the phase field function approximately, but this is sufficient for most applications.

When the Phase Field in Fluids interface is coupled to a fluid flow interface by means of The Two-Phase Flow, Phase Field Coupling Feature, conservation of the integral of ϕ using the nonconservative form can be improved provided that the discretization order of the phase field variables is equal to or lower than the order of the pressure.

Additional Sources of Free Energy

In some cases, the expression for the free energy can include other sources. It is possible to incorporate these by modifying Equation 11-16:

$$\psi = -\nabla \cdot \varepsilon^2 \nabla\phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial \phi} \tag{11-18}$$

where f is a user-defined free energy (SI unit: $\mathrm{J/m^3}$).

The expression for the external free energy must be manually differentiated with respect to ϕ and then entered into the $\partial f/\partial\phi$ field. In most cases, the external free energy is zero.

Initializing the Phase Field Function

If the study type Transient with Phase Initialization is used in the model, the phase field variable is first initialized so that it varies smoothly between zero and one over the interface. For this study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi}. The Time Dependent step then uses the initial condition for the phase field function according to the expression

$$\phi_0 = -\tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{\mathrm{wi}}}{\sqrt{2}\varepsilon}\right)$$

in Fluid 2. These expressions are based on a steady, analytic solution to Equation 11-15 and Equation 11-16 for a straight, nonmoving interface.

!	If the **Transient with Phase Initialization** ( ) study is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes is set to **Specify phase: Fluid 1 ($\phi = -1$)** and the other to **Specify phase: Fluid 2 ($\phi = 1$)**. The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

?	Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

Variables and Expressions

The physics interface defines the chemical potential, which can be rewritten in terms of the dependent variable ψ,

$$G = \frac{\lambda\psi}{\varepsilon^2}$$

and the surface tension force $\mathbf{F} = G\nabla\phi$.

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi = 0,5} \tag{11-19}$$

This variable is available in the physics interface as the interface normal `pf.intnorm`.

The mean curvature (SI unit: 1/m) of the interface can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

Reference for the Phase Field in Fluids Interface

1. P. Yue, C. Zhou, J.J. Feng, C.F. Ollivier-Gooch, and H.H. Hu, "Phase-field Simulations of Interfacial Dynamics in Viscoelastic Fluids Using Finite Elements with Adaptive Meshing," *J. Comp. Phys.*, vol. 219, pp. 47–67, 2006.

Theory for the Phase Field Thin-Film Flow Interfaces

The Phase Field Thin-Film Flow Interfaces' theory is described in this section:

- About the Phase Field Thin-Film Flow Method
- The Equations for the Phase Field Thin-Film Flow Method
- Conservative and Nonconservative Forms
- Additional Sources of Free Energy
- Initializing the Phase Field Function
- Variables and Expressions
- Reference for the Phase Field Thin-Film Flow Interfaces

About the Phase Field Thin-Film Flow Method

The phase field thin-film flow method offers an attractive alternative to more established methods for solving multiphase flow problems in narrow channels represented by a surface or an edge within the geometry. Instead of directly tracking the interface between two fluids, the interfacial layer is governed by a phase field variable, ϕ. The surface tension force is added to the momentum equation as a body force by multiplying the chemical potential of the system by the gradient of the phase field variable.

The evolution of the phase field variable is governed by the *Cahn–Hilliard equation*, which is a 4th-order PDE. The Phase Field Thin-Film Flow interface decomposes the Cahn–Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn–Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of two immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple two-phase flows, only the mixing energy is retained, which results in a rather simple expression for the free energy.

The free energy is a functional of a dimensionless phase field parameter, ϕ:

$$F(\phi, \nabla_t\phi, T) = \int\left(\frac{1}{2}\varepsilon^2\left|\nabla_t\phi\right|^2 + f(\phi, T)\right)dV = \int f_{\text{tot}}dV$$

where ε is a measure of the interface thickness. Equation 11-20 describes the evolution of the phase field parameter:

$$\frac{\partial\phi}{\partial t} + (\mathbf{u}\cdot\nabla_t)\phi = \nabla_t\cdot\gamma\nabla_t\left(\frac{\partial f_{\text{tot}}}{\partial\phi} - \nabla_t\cdot\frac{\partial f_{\text{tot}}}{\partial\nabla_t\phi}\right) \tag{11-20}$$

where f_{tot} (SI unit: J/m^3) is the total free energy density of the system, and $\mathbf{u}$ (SI unit: m/s) is the velocity field for the advection. The right-hand side of Equation 11-20 aims to minimize the total free energy with a relaxation time controlled by the mobility γ (SI unit: $\text{m}^3\cdot\text{s/kg}$).

The free energy density of an isothermal mixture of two immiscible fluids is the sum of the mixing energy and elastic energy. The mixing energy assumes the Ginzburg-Landau form:

$$f_{\text{mix}}(\phi, \nabla_t\phi) = \frac{1}{2}\lambda\left|\nabla_t\phi\right|^2 + \frac{\lambda}{4\varepsilon^2}(\phi^2 - 1)^2$$

where ϕ is the dimensionless phase field variable, defined such that the volume fraction of the components of the fluid are $(1+\phi)/2$ and $(1-\phi)/2$. The quantity λ (SI unit: N) is the mixing energy density and ε (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon} \tag{11-21}$$

The PDE governing the phase field variable is the Cahn–Hilliard equation:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla_t\phi = \nabla_t\cdot\gamma\nabla_t G \tag{11-22}$$

where G (SI unit: Pa) is the chemical potential and γ (SI unit: $\text{m}^3\cdot\text{s/kg}$) is the mobility. The mobility determines the time scale of the Cahn–Hilliard diffusion and must be large enough to retain a constant interfacial thickness but small enough so that the

convective terms are not overly damped. In COMSOL Multiphysics the mobility is determined by a mobility tuning parameter that is a function of the interface thickness $\gamma = \chi\varepsilon^2$. The chemical potential is:

$$G = \lambda\left[-\nabla_t^2\phi + \frac{\phi(\phi^2-1)}{\varepsilon^2}\right] \tag{11-23}$$

The Cahn–Hilliard equation forces ϕ to take a value of 1 or –1 except in a very thin region on the fluid-fluid interface. The Phase Field Thin-Film Flow interface breaks Equation 11-13 up into two second-order PDEs:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla_t\phi = \nabla_t\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla_t\psi \tag{11-24}$$

$$\psi = -\nabla_t\cdot\varepsilon^2\nabla_t\phi + (\phi^2-1)\phi \tag{11-25}$$

Conservative and Nonconservative Forms

If the velocity field is divergence free, that is, if

$$\nabla_t\cdot\mathbf{u} = 0 \tag{11-26}$$

the area (length for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the edges (nodes for 2D problems). To obtain exact numerical conservation in cases where Equation 11-26 is not fully satisfied, switch to the conservative form

$$\frac{\partial\phi}{\partial t} + \nabla_t\cdot\mathbf{u}\phi = \nabla_t\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla_t\psi$$

Using the conservative phase field form, exact numerical conservation of the integral of ϕ is obtained. However, the nonconservative form is better suited for numerical calculations and usually converges more easily. The nonconservative form, which is the default form, only conserves the integral of the phase field function approximately, but this is sufficient for most applications.

When the Phase Field Thin-Film Flow interface is coupled to a Thin-Film Flow interface by means of The Two-Phase Thin-Film Flow, Phase Field Coupling Feature, conservation of the integral of ϕ using the nonconservative form can be improved

provided that the discretization order of the phase field variables is equal to or lower than the order of the film pressure.

Additional Sources of Free Energy

In some cases, the expression for the free energy can include other sources. It is possible to incorporate these by modifying Equation 11-25:

$$\psi = -\nabla_t \cdot \varepsilon^2 \nabla_t \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial \phi} \tag{11-27}$$

where f is a user-defined free energy (SI unit: $\mathrm{J/m^3}$).

The expression for the external free energy must be manually differentiated with respect to ϕ and then entered into the $\partial f/\partial\phi$ field. In most cases, the external free energy is zero.

Initializing the Phase Field Function

See Initializing the Phase Field Function.

Variables and Expressions

The physics interface defines the chemical potential, which can be rewritten in terms of the dependent variable ψ,

$$G = \frac{\lambda\psi}{\varepsilon^2}$$

and the surface tension force $\mathbf{F} = G\nabla_t\phi$.

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \left.\frac{\nabla_t\phi}{|\nabla_t\phi|}\right|_{\phi = 0{,}5} \tag{11-28}$$

This variable is available in the physics interface as the interface normal `pftff.intnorm`.

The mean curvature (SI unit: 1/m) of the interface can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

Reference for the Phase Field Thin-Film Flow Interfaces

See Reference for the Phase Field in Fluids Interface.

Theory for the Ternary Phase Field Interface

The Phase Field Thin-Film Flow Interfaces theory is described in this section:

- About the Phase Field Method
- The Equations of the Ternary Phase Field Method
- Reference for the Phase Field in Fluids Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the separating interface is identified as the region across which the phase field variables of the two adjacent phases varies between its two limiting values. The surface tension force is added to the Navier–Stokes equations as a body force by multiplying the chemical potentials of the phases by the gradient of the corresponding phase field variable.

The evolution of each phase field variable is governed by the *Cahn–Hilliard equation*, which is a 4th-order PDE. The Ternary Phase Field interface decomposes each Cahn–Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn–Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple three-phase flows, only the mixing energy is retained.

The Equations of the Ternary Phase Field Method

The ternary phase field model implemented in COMSOL is based the work of Boyer and co-workers in Ref. 2. The model is designed in order to study the evolution of the three immiscible phases, denoted phase A, phase B, and phase C, respectively. Each phase is represented by a phase field variable ϕ, which takes values between 0 and 1. The phase field variables satisfies the constraint

$$\sum_{i = \mathrm{A}, B, C} \phi_i = 0 \tag{11-29}$$

and density of each phase is assumed to be constant. This implies that the phase field variable corresponds directly to the volume fraction of the phase in question.

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$\begin{aligned} F = {} & \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 + \\ & \phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2 \end{aligned} \tag{11-30}$$

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase i and j, and the capillary parameters Σ_i are defined as

$$\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk} \tag{11-31}$$

and Λ is a function or parameter specifying the additional free bulk energy. By default Λ is zero. In this case it can be seen that the free energy in Equation 11-30 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

The Cahn–Hilliard equations to be solved for each phase $p = A, B, C$ are

$$\begin{aligned} \frac{\partial\phi_i}{\partial t} + \frac{\partial u_j\phi_i}{\partial x_j} &= \frac{\partial}{\partial x_j}\left(\frac{M_0}{\Sigma_i}\frac{\partial\eta_i}{\partial x_j}\right) \\ \eta_i = \frac{4\Sigma_{\mathrm{T}}}{\varepsilon}\sum_{j \neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial\phi_i} - \frac{\partial F}{\partial\phi_j}\right)\right) &- \frac{3}{4}\varepsilon\Sigma_j\frac{\partial}{\partial x_j}\left(\frac{\partial\eta_i}{\partial x_j}\right) \end{aligned} \tag{11-32}$$

It can be noted that the Cahn–Hilliard equation is originally a 4th-order PDE. In COMSOL Multiphysics, that PDE is split up into two second-order PDEs by introducing an additional dependent variable, the generalized potential η, one for each phase. In order to satisfy Equation 11-30, two sets of the equations shown in Equation 11-32 are solved, those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 11-30.

In Equation 11-32 ε (SI unit: 1/m) is a parameter controlling the interface thickness, M_0 (SI unit: m^3/s) is a molecular mobility parameter, and the parameter Σ_{T} is defined as

$$\frac{3}{\Sigma_{\mathrm{T}}} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \tag{11-33}$$

Reference for the Ternary Phase Field Interface

2. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar, and M. Quintard, "Cahn–Hilliard/Navier–Stokes model for the simulation of three-phase flows", *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

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5. A. G. Gaonkar, "Interfacial Tensions of Vegetable Oil/Water Systems: Effect of Oil Purification", *J. Am. Oil Chem. Soc.*, vol. 66, no. 8, pp. 1090-1092, 1989.

12

Glossary

This Glossary of Terms contains application-specific terms used in the CFD Module software and documentation. For finite element modeling terms, mathematical terms, and geometry and CAD terms, see the glossary in the *COMSOL Multiphysics Reference Manual*. For references to more information about a term, see the index.

Glossary of Terms

algebraic yPlus turbulence model Low-Reynolds number, algebraic turbulence model that solves for the wall distance, y^+ (in viscous units).

anisotropy Directional dependence. Is often obtained from homogenization of regular structures, for example, monolithic structures in tubular reactors.

Boussinesq approximation An approximate method to include buoyancy effects, for which the density variation is only taken into account in the buoyancy term.

Brinkman equations A set of equations extending Darcy's law in order to include transport of momentum through shear in porous media flow.

boundary layer Region in a fluid close to a solid surface. This region is characterized by large gradients in velocity and other properties. In turbulent flow it is often treated with approximate methods because of the difficulty to resolve the large gradients.

bubbly flow Flow with gas bubbles dispersed in a liquid.

conjugate heat transfer heat transfer that takes place in both a solid and a fluid.

creeping flow Models the Navier-Stokes equations without the contribution of the inertial term. This is often referred to as *Stokes flow* and is applicable when viscous flow dominates, such as in very small channels or microfluidic devices.

crosswind diffusion A numerical technique for stabilization of convection-dominated PDEs by artificially adding diffusion perpendicular to the direction of the streamlines. It reduces oscillations near sharp gradients.

Darcy's law Equation that gives the velocity vector as proportional to the pressure gradient. Often used to describe flow in porous media.

Euler flow Flow of an inviscid fluid. Often used to approximate high speed compressible flows.

Euler-Euler model A two-phase flow model that treats both phases as interpenetrating continua.

Fick's laws The first law states that the diffusive flux of a solute infinitely diluted in a solvent is proportional to its concentration gradient. The second law introduces the first law into a differential material balance for the temporal evolution of the solute.

fluid-structure interaction (FSI) When a fluid flow affects the deformation of a solid object and vice versa.

fully developed laminar flow Laminar flow along a channel or pipe that only has velocity components in the streamwise direction. The velocity profile does not change downstream.

Hagen-Poiseuille equation See *Poiseuille's law*.

heterogeneous reaction Reaction that takes place at the interface between two phases.

homogeneous reaction Reaction that takes place in the bulk of a solution.

intrinsic volume averages The physical properties of the fluid, such as density, viscosity, and pressure.

k-ε turbulence model A two-equation RANS model that solves for the turbulent kinetic energy, k, and the dissipation of turbulence kinetic energy, ε. Utilizes wall functions to describe the flow close to solid walls.

k-ω turbulence model A two-equation RANS model that solves for the turbulent kinetic energy, k, and the specific dissipation rate, ω. Utilizes wall functions to describe the flow close to solid walls.

L-VEL turbulence model Low-Reynolds number, algebraic turbulence model that solves for the tangential velocity near walls, u^+ (in viscous units).

law of the wall See *wall function*.

low-Reynolds k-ε turbulence model Two-equation RANS model that solves for the turbulence kinetic energy, k, and the dissipation of turbulence kinetic energy, ε. Includes damping functions to be able to describe regions with low Reynolds numbers, for example close to solid walls.

low Reynolds number The region close to the wall where viscous effects dominate.

Mach number Dimensionless number equal to the flow velocity over the speed of sound. Compressible effects because of the flow speed can be neglected for Mach number less than 0.3.

multiphase flow Flow with more than one phase.

Navier–Stokes equations The momentum balance equation for a Newtonian fluid coupled to the equation of continuity. The meaning of the term originally only referred to the momentum balance but it is here used in the more general context.

Newtonian fluid A fluid for which the stress is proportional to the rate of strain. Many common fluids such as water and air are Newtonian.

non-Newtonian fluid A fluid for which the stress is *not* proportional to the rate of strain. Blood and suspensions of polymers are examples of non-Newtonian fluids.

Poiseuille's law Equation stating that the mass rate of flow in a tube is proportional to the pressure difference per unit length and to the fourth power of the tube radius. The law is valid for fully developed laminar flow.

pressure work Describes the reversible conversion of work, performed by the pressure in a fluid, into heat.

RANS Reynolds-averaged Navier–Stokes; implying that a time-averaging operation has been performed on the equations of motion. The Reynolds' stresses (correlations between fluctuating velocity components) obtained from this averaging operation have to be obtained from an additional set of equations — a closure. Turbulence models like the k-ε and Spalart–Allmaras models constitute closures to the RANS equations.

Reynolds number A dimensionless number that describes the relative importance between inertia and viscous effects. Flow at high Reynolds number have a tendency to undergo transition to turbulence.

Soret effect Mass diffusion due to temperature gradients in multicomponent mixtures.

Spalart–Allmaras turbulence model A one-equation turbulence model that solves for the undamped turbulent kinematic viscosity, $\tilde{\nu}_T$.

SST turbulence model The Shear Stress Transport model is a two-equation turbulence model combining the k-ω model in the near-wall region with the k-ε model in the free stream. The SST model is a low-Reynolds number model requiring high resolution near walls. The dependent variables are the turbulent kinetic energy, k, and the turbulent dissipation rate, ω.

Stokes flow See *creeping flow*.

streamline diffusion A numerical technique for stabilization of convection-dominated PDEs by artificially adding upwinding in the streamline direction.

superficial volume averages The flow velocities, which correspond to a unit volume of the medium including both pores and matrix. They are sometimes called Darcy velocities, defined as volume flow rates per unit cross section of the medium.

thin-film flow Flow in very thin regions where the it can be assumed to always have a fully developed profile.

viscous heating The heat irreversibly generated from work by viscous friction in a fluid.

wall function Semi-empirical expression for the boundary-layer flow used in turbulence models. Often based on the assumption of negligible variations in the pressure gradient tangential to the surface.

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