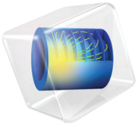

# Microfluidics Module

## User's Guide

5.3

COMSOL

## Microfluidics Module User's Guide

Version: COMSOL 5.3

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# 1

# Introduction

This guide describes the Microfluidics Module, an optional add-on package that extends the COMSOL Multiphysics® modeling environment with customized physics interfaces for microfluidics.

This chapter introduces you to the capabilities of this 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.

In this chapter:

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

# About the Microfluidics Module

In this section:

- About Microfluidics
- About the Microfluidics Module
- The Microfluidics Module Physics Interface Guide
- Coupling to Other Physics Interfaces
- The Microfluidics Module Study Capabilities by Physics Interface
- Common Physics Interface and Feature Settings and Nodes
- The Liquids and Gases Materials Database
- Where Do I Access the Documentation and Application Libraries?

## *About Microfluidics*

The field of *microfluidics* evolved as engineers and scientists explored new avenues to exploit the fabrication technologies developed by the microelectronics industry. These technologies enabled complex micron and submicron structures to be integrated with electronic systems and batch fabricated at low cost. Mechanical devices fabricated using these technologies have become known as microelectromechanical systems (MEMS), whilst fluidic devices are commonly referred to as microfluidic systems or “lab-on-a-chip” devices. A proper description of these microsystems usually requires multiple physical effects to be incorporated.

At the microscale different physical effects become important to those dominant at macroscopic scales. Properties that scale with the volume of the system (such as inertia) become comparatively less important than those that scale with the surface area of the system (such as viscosity and surface tension). Fluid flow is therefore usually laminar and chemical migration is often limited by diffusion. Electrokinetic effects become important as the electric double layers present at interfaces in the system interact with external applied fields. As systems are further miniaturized, the mean free path of the fluid can become comparable to the size of the system and rarefaction effects become important. At moderate Knudsen numbers (the Knudsen number is the ratio of the mean free path to the system size), it is still possible to use the Navier-Stokes equations to solve the flow, however special slip boundary conditions are required.

Research activity in microfluidics is changing medical-diagnostic processes such as DNA analysis, and it is spurring the development of successful commercial products.

The Microfluidics Module has a range of tools to address the specific challenges of modeling micro- and nanoscale flows. In addition to the standard tools for modeling fluid flow, interfaces between fluids can be modeled by the Level Set, Phase Field, and Moving Mesh interfaces, enabling the modeling of surface tension and multiphase flow at the microscale. For dilute species, chemical transport and reactions can be modeled. COMSOL Multiphysics also has tools to model the transport and reactions of concentrated species, but the Chemical Reaction Engineering Module is required for these physics interfaces.

Tools to address the flow of fluids within porous media are also included as well as a physics interface to model moderately rarefied gas flows (the Slip Flow interface).

## *About the Microfluidics Module*

The Microfluidics Module is a collection of tailored physics interfaces for the simulation of microfluidic devices. It has a range of tools to address the specific challenges of modeling micro- and nanoscale flows. Physics interfaces that address laminar flow, multiphase flow, flow in porous media, and moderately rarefied flow (the Slip Flow interface) are available. Enhanced capabilities to treat chemical reactions between dilute species are also included. In addition to the standard tools for modeling fluid flow, interfaces between fluids can be modeled by the Level Set, Phase Field, and Moving Mesh interfaces, making it possible to model surface tension and multiphase flow at the microscale.

The Microfluidics Module Applications Libraries and supporting documentation explain how to use the physics interfaces to model a range of microfluidic devices.

## *The Microfluidics Module Physics Interface Guide*

The physics interfaces in the Microfluidics Module form a complete set of simulation tools, which 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

Microfluidics Module are listed in the table. The functionality of the COMSOL Multiphysics base package is given in the *COMSOL Multiphysics Reference Manual*.

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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.

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| PHYSICS INTERFACE | ICON | TAG | SPACE DIMENSION | AVAILABLE PRESET STUDY TYPE |
|---|---|---|---|---|
| **Chemical Species Transport** | | | | |
| Transport of Diluted Species[1] | | tds | all dimensions | stationary; time dependent |
| Transport of Diluted Species in Porous Media | | tds | all dimensions | stationary; time dependent |
| **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 |
| **Multiphase Flow** | | | | |
| *Two-Phase Flow, Level Set* | | | | |
| Laminar Two-Phase Flow, Level Set | | — | 3D, 2D, 2D axisymmetric | transient with phase initialization |

| PHYSICS INTERFACE | ICON | TAG | SPACE DIMENSION | AVAILABLE PRESET STUDY TYPE |
|---|---|---|---|---|
| *Two-Phase Flow, Phase Field* | | | | |
| Laminar Two-Phase Flow, Phase Field | | — | 3D, 2D, 2D axisymmetric | transient with phase initialization |
| *Three-Phase Flow, Phase Field* | | | | |
| Laminar, Three-Phase Flow, Phase Field | | — | 3D, 2D | time dependent |
| *Two-Phase Flow, Moving Mesh* | | | | |
| Laminar Two-Phase Flow, Moving Mesh | | tpfmm | 3D, 2D, 2D axisymmetric | 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 |
| Free and Porous Media Flow | | fp | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| **Rarefied Flow** | | | | |
| Slip Flow | | slpf | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| **Mathematics** | | | | |
| **Moving Interface** | | | | |
| Level Set | | ls | all dimensions | transient with phase initialization |
| Phase Field | | pf | all dimensions | time dependent; transient with phase initialization |

| PHYSICS INTERFACE | ICON | TAG | SPACE DIMENSION | AVAILABLE PRESET STUDY TYPE |
|---|---|---|---|---|
| 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.

## *Coupling to Other Physics Interfaces*

The Microfluidics Module connects to COMSOL Multiphysics and other add-on modules in the COMSOL Multiphysics product line. Table 1-1 summarizes the most important microfluidics couplings and other common devices you can model.

The *Microfluidics* column lists transport phenomena that are key issues in, for example, lab-on-a-chip type devices.

This list is only the tip of the iceberg — an overview of the most important applications where you can use the Microfluidics Module. In your hands, the multiphysics combinations and applications are unlimited.

TABLE 1-1: EXAMPLES OF COUPLED PHENOMENA AND DEVICES YOU CAN MODEL USING THE MICROFLUIDICS MODULE

| | MICROFLUIDICS |
|---|---|
| PHENOMENA/ COUPLING | Pressure-driven flow |
| | Chemical Reactions in two-phase flow |
| | Dielectrophoresis |
| | Electroosmotic flow |
| | Electrophoresis |
| | Electrothermal flow |
| | Electrowetting |
| | Magnetophoresis |
| | Mass transport using diffusion, migration, and convection |
| | Slip Flow |
| DEVICES | Lab-on-a-chip devices |
| | Microfluidic channels |
| | Microreactors |
| | Micromixers |
| | MEMS heat exchangers |
| | Nonmechanical pumps and valves |

## *The Microfluidics Module Study Capabilities by Physics Interface*

Table 1-2 lists the Preset Studies available for each physics interface specific to this module.

When using the axisymmetric interfaces, the horizontal axis represents the *r* direction and the vertical axis the *z* direction. The geometry must be created in the right half-plane (that is, only for positive *r*).

Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

TABLE 1-2: MICROFLUIDICS MODULE DEPENDENT VARIABLES AND PRESET STUDY AVAILABILITY

| **PHYSICS INTERFACE** | **NAME** | **DEPENDENT VARIABLES** | **PRESET STUDIES*** | | |
|---|---|---|---|---|---|
| | | | **STATIONARY** | **TIME DEPENDENT** | **TRANSIENT WITH INITIALIZATION** |
| **CHEMICAL SPECIES TRANSPORT** | | | | | |
| Transport of Diluted Species | tds | $c$ | √ | √ | |
| Transport of Diluted Species in Porous Media | tds | $c$ | √ | √ | |
| **FLUID FLOW>RAREFIED FLOW** | | | | | |
| Slip Flow | slpf | $u, v, w, p, T$ | √ | √ | |
| **FLUID FLOW>SINGLE-PHASE FLOW** | | | | | |
| Laminar Flow | spf | $u, v, w, p$ | √ | √ | |
| Creeping Flow | spf | $u, v, w, p$ | √ | √ | |
| **FLUID FLOW>MULTIPHASE FLOW** | | | | | |
| Laminar Two-Phase Flow, Level Set | tpf | $u, v, w, p, \phi$ | | | √ |

TABLE 1-2: MICROFLUIDICS MODULE DEPENDENT VARIABLES AND PRESET STUDY AVAILABILITY

| **PHYSICS INTERFACE** | **NAME** | **DEPENDENT VARIABLES** | **PRESET STUDIES*** | | |
|---|---|---|---|---|---|
| | | | **STATIONARY** | **TIME DEPENDENT** | **TRANSIENT WITH INITIALIZATION** |
| Laminar Two-Phase Flow, Phase Field | tpf | $u, v, w, p, \phi, \psi$ | | | √ |
| Laminar Two-Phase Flow, Moving Mesh | tpfmm | $u, v, w, p$ | | √ | |
| **FLUID FLOW>POROUS MEDIA AND SUBSURFACE FLOW** | | | | | |
| Brinkman Equations | br | $u, v, w, p$ | √ | √ | |
| Darcy's Law | dl | $u, v, w, p$ | √ | √ | |
| Free and Porous Media Flow | fp | $u, v, w, p$ | √ | √ | |
| **MATHEMATICS** | | | | | |
| Level Set | ls | $\phi$ | | | √ |
| Phase Field | pf | $\phi, \psi$ | | | √ |

* Custom studies are also available based on the physics interface.

## *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 2-3 for links to common sections and Table 2-4 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 Microfluidics Module includes an additional **Liquids and Gases** material database with temperature-dependent fluid dynamic and thermal properties.

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

## *Where Do I Access the Documentation and Application Libraries?*

A number of internet 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 (as long as you have a license), 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 about 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 many of the features on the GUI. 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.
- On the main toolbar, click the **Help** ( ? ) button.
- From the main menu, select **Help>Help**.

### *Opening the Documentation Window*

Win

To open the **Documentation** window:

- Press Ctrl+F1.
- From the **File** menu select **Help>Documentation** ( 📘 ).

Mac

Linux

To open the **Documentation** window:

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

### THE APPLICATION LIBRARIES WINDOW

Each application includes documentation with the theoretical background and step-by-step instructions to create a model application. The applications are available in COMSOL as MPH-files that you can open for further investigation. You can use the step-by-step instructions and the actual applications as a template for your own modeling and applications. In most models, SI units are used to describe the relevant properties, parameters, and dimensions in most examples, 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 application and its properties, including options to open it or a PDF document.

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The Application Libraries Window in the *COMSOL Multiphysics Reference Manual*.

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*Opening the Application Libraries Window*

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

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Win

- From the **Home** toolbar, **Windows** menu, click ( ) **Applications Libraries**.
- From the **File** menu select **Application Libraries**.

To include the latest versions of model examples, from the **File>Help** menu, select ( ) **Update COMSOL Application Library**.

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Mac

Linux

Select **Application Libraries** from the main **File>** or **Windows>** menus.

To include the latest versions of model examples, from the **Help** menu select ( ) **Update COMSOL Application Library**.

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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 are sent to you by email.

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| Support Knowledge Base | www.comsol.com/support/knowledgebase |

# Overview of the User's Guide

The *Microfluidics Module User's Guide* gets you started with modeling microfluidic systems using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions how to use COMSOL Multiphysics in general are included with the *COMSOL Multiphysics Reference Manual*.

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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.

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### TABLE OF CONTENTS, GLOSSARY, AND INDEX

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

### MODELING IN MICROFLUIDICS

The Microfluidic Modeling chapter familiarizes you with modeling procedures useful when working with this module. Topics include Dimensionless Numbers in Microfluidics, Modeling Microfluidic Fluid Flows, Modeling Coupled Phenomena in Microfluidics, and Modeling Rarefied Gas Flows.

### THE FLUID FLOW BRANCH INTERFACES

There are several fluid flow interfaces available. The various types of momentum transport that you can simulate includes laminar and creeping flow, multiphase two-phase flow, and flow in porous media. Every section describes the applicable physics interfaces in detail and concludes with the underlying interface theory.

#### *Single-Phase Flow*

Single-Phase Flow Interfaces chapter describes the Laminar Flow and Creeping Flow interfaces.

#### *Multiphase Flow Two-Phase Flow*

Multiphase Flow, Two-Phase Flow Interfaces chapter describes the Laminar Flow, Two-Phase Flow Level Set and Phase Field interfaces as well as the Laminar Flow, Two-Phase Flow, Moving Mesh interface. Some multiphase flow is described using the Phase Field and Level Set interfaces found under Mathematics, Moving Interfaces branch. In this module these physics are already integrated into the relevant physics interfaces.

#### *Porous Media and Subsurface Flow*

Porous Media Flow Interfaces chapter describes the Darcy's Law, Brinkman Equations, and Free and Porous Media Flow interfaces.

#### *Rarefied Flow*

Rarefied Flow Interface chapter describes the Slip Flow interface, including the underlying theory.

### THE CHEMICAL SPECIES TRANSPORT BRANCH INTERFACES

The transport and conversion of material is denoted as chemical species transport. Chemical Species Transport Interfaces chapter describes the Transport of Diluted Species and the Transport of Diluted Species in Porous Media as well as the underlying theory.

# 2

# Microfluidic Modeling

This chapter gives an overview of the physics interfaces available for modeling microfluidic flows and provides guidance on choosing the appropriate physics interface for a specific problem.

In this chapter:

# Physics and Scaling in Microfluidics

Microfluidic flows occur on length scales that are orders of magnitude smaller than macroscopic flows. Manipulation of fluids at the microscale has a number of advantages — typically microfluidic systems are smaller, operate faster, and require less fluid than their macroscopic equivalents. Energy inputs and outputs are also easier to control (for example, heat generated in a chemical reaction) because the surface-to-area volume ratio of the system is much greater than that of a macroscopic system.

In general, as the length scale ($L$) of the fluid flow is reduced, properties that scale with the surface area of the system become comparatively more important than those that scale with the volume of the flow (see Table 2-1). This is apparent in the fluid flow itself as the viscous forces, which are generated by shear over the isovelocity surfaces (scaling as $L^2$), dominate over the inertial forces (which scale volumetrically as $L^3$). The Reynolds number ($\mathrm{Re}$), which characterizes the ratio of these two forces, is typically low, so the flow is laminar. In many cases the creeping (Stokes) flow regime applies ( $\mathrm{Re} \ll 1$ ). The section Single-Phase Flow describes microfluidic fluid flows in greater detail.

When multiple phases are present surface tension effects become important relative to gravity and inertia at small length scales. The Laplace pressure, capillary force, and Marangoni forces all scale as $1/L$. The section Multiphase Flow gives more information on modeling flows involving several phases.

Flow through porous media can also occur on microscale geometries. Because the permeability of a porous media scales as $L^2$ (where $L$ is the average pore radius) the flow is often friction dominated when the pore size is in the micron range and Darcy's law can be used. For intermediate flows this module also provides a physics interface to model flows where Brinkman equation is appropriate. For more information see Porous Media Flow.

At the microscale a range of electrohydrodynamic effects can be exploited to influence the fluid flow. The electric field strength for a given applied voltage scales as $1/L$, making it easier to apply relatively large fields to the fluid with moderate voltages. In electroosmosis the uncompensated ions in the charged electric double layer (EDL) present on the fluid surfaces are moved by an electric field, causing a net fluid flow. Electrophoretic and dielectrophoretic forces on charged or polarized particles in the fluid can be used to induce particle motion, as can diamagnetic forces in the case of magnetophoresis. The manipulation of contact angles by the electrowetting phenomena is also easy in microscale devices. The section Electrohydrodynamics explains how to model these phenomena in detail.

TABLE 2-1: SCALING OF VARIOUS PHYSICAL PHENOMENA WITH LENGTH (L) AND THE CONSEQUENCES FOR MICROFLUIDIC DEVICES

| **PROPERTY** | **LENGTH SCALING** | **CONSEQUENCES** |
|---|---|---|
| Volume | $L^3$ | Surface related properties increase in importance relative to volumetric properties, Surface area to volume ratios are high. |
| Area | $L^2$ | |
| Inertial Forces | $L^3$ | Viscosity dominates over inertia, flow is laminar or creeping. Absence of convection makes mixing difficult. |
| Viscous Forces | $L^2$ | |
| Laplace Pressure | $L^{-1}$ | Surface tension effects become dominant in two phase flows. |
| Capillary Force | $L^{-1}$ | |
| Permeability of Porous media | $L^2$ | Darcy's law usually applies. |
| Diffusion Time Scale | $L^2$ | Diffusive mixing possible (although still much slower than convection). |
| Electric Field (at constant applied voltage) | $L^{-1}$ | Possibility of using a range of electrokinetic effects to drive the flow. |
| Knudsen Number | $L^{-1}$ | Microscale gas flows are usually rarefied. |

Laminar flows make mixing particularly difficult, so mass transport is often diffusion limited. The diffusion time scales as $L^2$, but even in microfluidic systems diffusion is often a slow process. This has implications for chemical transport and hence reactions within microfluidic systems. Chemical Transport and Reactions describes how to model diffusion-based transport and chemical reactions in microfluidics.

As the length scale of the flow becomes comparable to intermolecular length scale, more complex kinetic effects become important. For gases the ratio of the molecular mean free path to the flow geometry size is given by the Knudsen number (Kn). Clearly, Kn scales as $1/L$. For $\mathrm{Kn} < 0.01$, fluid flow is usually well described by the Navier-Stokes equations with no-slip boundary conditions. In the slip flow regime ($0.01 < \mathrm{Kn} < 0.1$) appropriate slip boundary conditions can be used with the Navier-Stokes equations to describe the flow away from the boundary (see Slip Flow). At Knudsen numbers above 0.1 a fully kinetic approach is required. Flows in this regime can be modeled using tools from the Molecular Flow Module.

The next section describes the importance of Dimensionless Numbers in Microfluidics, which are frequently used in transport equations.

| | |
|---|---|
| 💡 | The Free Molecular Flow and Transitional Flow interfaces are available in the Molecular Flow Module. |

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

# Dimensionless Numbers in Microfluidics

Information about the dominant physics in a microfluidics problem is contained in many of the dimensionless numbers that are used to characterize the flow. When using the finite element method, dimensionless numbers defined on the element or "cell" level can contain important information about the numerical stability of the problem (the term "cell" is carried over from the finite volume method in this context). This section includes information about the dimensionless numbers that are relevant to microfluidic flows.

In this section:

- Dimensionless Numbers Important for Solver Stability
- Other Dimensionless Numbers

## *Dimensionless Numbers Important for Solver Stability*

When solving a microfluidics problem numerically there are two critical dimensionless numbers to consider in terms of solver stability. These numbers are:

- The Reynolds number (Re)
- The Peclet number (Pe)

Each of these numbers is defined in Table 2-2. Both the Reynolds number and the Peclet number are associated with the relative importance of convective terms in the corresponding partial differential equation. The *Peclet number* describes the importance of convection in relation to diffusion (for either heat or mass transfer), and the *Reynolds number* describes the importance of the "convective" inertia term in relation to viscosity in the Navier-Stokes equations themselves.

Both the Reynolds number and the Peclet number can be defined on the "cell" or element level. As they are defined in COMSOL Multiphysics numerical instabilities can arise when the cell Reynolds or Peclet number is greater than one. These instabilities are usually manifested as spurious oscillations in the solution. Taking the Peclet number as an example, oscillations can occur when the cell Peclet number is greater than one in the following circumstances:

- A Dirichlet boundary condition can lead to a solution containing a steep gradient near the boundary, forming a boundary layer. If the mesh cannot resolve the boundary layer, this creates a local disturbance.
- A space-dependent initial condition that the mesh does not resolve can cause a local initial disturbance that propagates through the computational domain.
- A small initial diffusion term close to a nonconstant source term or a nonconstant Dirichlet boundary condition can result in a local disturbance.

In theory the grid can be refined to bring the cell Reynolds or Peclet number below one, although this is often impractical for many problems. Several stabilization techniques are included, which enable problems with larger cell Reynolds or Peclet numbers to be solved. At the crudest level additional numerical diffusion can be added to the problem to improve its stability. This is achieved by selecting **Isotropic Diffusion** under **Inconsistent Stabilization** for any physics interface.

The stabilization options are visible when the **Show** button ( 👁 ) is clicked and **Stabilization** is selected.

This method is termed “inconsistent” as a solution to the problem without numerical diffusion is not necessarily a solution to the problem with diffusion. COMSOL Multiphysics also has consistent stabilization options. A consistent stabilization technique reduces the numerical diffusion added to the problem as the solution approaches the exact solution. Both streamline diffusion and crosswind diffusion are available. Streamline diffusion adds numerical diffusion along the direction of the flow velocity (that is, the diffusion is parallel to the streamlines). Crosswind diffusion adds diffusion in the direction orthogonal to the velocity.

Generally it is best to use consistent stabilization where possible. If convergence problems are still encountered, inconsistent stabilization can be used with a parametric or time-dependent solver that slowly eliminates this term.

- Stabilization and Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*
- Other Dimensionless Numbers

TABLE 2-2: IMPORTANT DIMENSIONLESS NUMBERS RELATED TO THE STABILITY OF VARIOUS MICROFLUIDIC PROBLEMS.

| **DIMENSIONLESS NUMBER** | **SYMBOL** | **GLOBAL DEFINITION** | **CELL DEFINITION** | **NOTES** |
|---|---|---|---|---|
| Reynolds number | $\mathrm{Re}$ | $\mathrm{Re} = \frac{\rho v L}{\mu}$ | $\mathrm{Re}^c = \frac{\rho v h}{2\mu}$<br>`spf.cellRe` | Ratio of inertial forces to viscous forces.<br>Laminar flow applies:<br>$\mathrm{Re} < 10^3$<br>Creeping flow applies:<br>$\mathrm{Re} \ll 1$<br>Stabilization required:<br>$\mathrm{Re}^c > 1$ |
| Peclet number (Heat Flow) | $Pe$ | $\mathrm{Pe} = \frac{\rho c_p v L}{\kappa}$ | $\mathrm{Pe}^c = \frac{\rho c_p v h}{2\kappa}$<br>`spf.cellPe` | Ratio of heat convection to thermal diffusivity,<br>$\alpha = \kappa/(\rho c_p)$.<br>Stabilization required:<br>$\mathrm{Pe}^c > 1$ |
| Peclet number (Mass Transport) | $\mathrm{Pe}$ | $\mathrm{Pe} = \frac{vL}{D}$ | $\mathrm{Pe}^c = \frac{vh}{2D}$ | Ratio of concentration convection to diffusion.<br>Stabilization required:<br>$\mathrm{Pe}^c > 1$ |

Symbol definitions: $v$ is the characteristic velocity or cell velocity, r is the fluid density, $L$ is the characteristic length scale for the problem, $\mu$ is the fluid viscosity, $h$ is the element size, $c_p$ is the heat capacity at constant pressure, $\kappa$ is the thermal conductivity, and $D$ is the diffusion constant. For anisotropic diffusion or conductivity an appropriate average is computed. The variables names assume the default name spf.

### *Other Dimensionless Numbers*

A number of other dimensionless numbers are useful for describing fluid flows on the microscale. These numbers are summarized in Table 2-3.

TABLE 2-3: DIMENSIONLESS NUMBERS USEFUL FOR CHARACTERIZING MICROFLUIDIC FLOWS.

| DIMENSION LESS NUMBER | SYMBOL | DEFINITION | NOTES |
|---|---|---|---|
| *Bond number/ Eötvös number* | $\mathrm{Bo}$<br>$\mathrm{Eo}$ | $\left.\begin{matrix}\mathrm{Bo}\\ \mathrm{Eo}\end{matrix}\right\} = \frac{\rho g L^2}{\sigma}$ | Ratio of surface tension forces to body forces (usually gravity) for two-phase flow. Density can refer to density difference when considering buoyancy. At high Bond numbers surface tension has a minimal effect on the flow, ($\mathrm{Bo} \gg 1$), at low Bond numbers, surface tension dominates ($\mathrm{Bo} < 1$). |
| *Capillary number* | $\mathrm{Ca}$ | $\mathrm{Ca} = \frac{\mu v}{\sigma}$ | Ratio of viscous forces to surface tension for two phase flow. At low capillary numbers ($\mathrm{Ca} < 10^{-5}$) flow in porous media is dominated by surface tension. |
| *Dukhin number* | $\mathrm{Du}$ | $\mathrm{Du} = \frac{K^{\sigma}}{K^{B}}$ | Ratio of the surface conductivity contribution to the fluid bulk electrical conductivity contribution in electrokinetic phenomena. For low Dukhin numbers ($\mathrm{Du} \ll 1$), surface conductivities can be neglected when modeling electrokinetic flows. |
| *Knudsen number* | $\mathrm{Kn}$ | $\mathrm{Kn} = \frac{\lambda}{L}$ | Ratio of the gas mean free path to the characteristic length scale. Continuum flow occurs when Kn<0.01, slip flow occurs in the range 0.01<Kn<0.1, transitional flow occurs in the range 0.1<Kn<10 and Free Molecular Flow occurs when Kn>10. For more details see Modeling Rarefied Gas Flows. |
| *Mach number* | $\mathrm{Ma}$ | $\mathrm{Ma} = \frac{v}{a}$ | Ratio of the convective speed to the speed of sound in the medium. The Laminar Flow interface in the Microfluidics Module can handle compressible flows with $\mathrm{Ma} < 0{,}3$. For higher Mach number flows the CFD Module is required. |

Symbol definitions: $\rho$ is the fluid density, $g$ is the body force acceleration (usually the acceleration due to gravity), $L$ is the characteristic length scale for the problem, $\sigma$ is the surface tension coefficient, $\mu$ is the fluid viscosity, v is the characteristic velocity, $K^{\sigma}$ is the surface conductivity, $K^{B}$ is the bulk conductivity, $\lambda$ is the mean free path, $\alpha$ is the thermal diffusivity ($\alpha=\kappa/(\rho c_p)$), $c_p$ is the heat capacity at constant pressure, $\kappa$ is the thermal conductivity, and $T$ is the absolute temperature ($\Delta T$ is the characteristic temperature difference).

TABLE 2-3: DIMENSIONLESS NUMBERS USEFUL FOR CHARACTERIZING MICROFLUIDIC FLOWS.

| **DIMENSION LESS NUMBER** | **SYMBOL** | **DEFINITION** | **NOTES** |
|---|---|---|---|
| *Marangoni number* | Mg | $\mathrm{Mg} = \frac{d\sigma}{dT}\frac{L\Delta T}{\mu\alpha}$ | Ratio of thermal surface tension forces to viscous forces. In the low Marangoni number range ($\mathrm{Mg} \ll 1000$) viscous forces dominate over surface tension gradients. |
| *Ohnesorge /Laplace /Surataman numbers* | Oh<br>La<br>Su | $\mathrm{Oh} = \frac{\mu}{\sqrt{\rho\sigma L}}$<br>$\left.\begin{matrix}\mathrm{La}\\ \mathrm{Su}\end{matrix}\right\} = \frac{1}{Oh^2}$ | Relates the inertial and surface tension forces to the viscous forces. Used to describe the breakup of liquid jets and sheets: at low Ohnesorge and Reynolds numbers the Rayleigh instability occurs, at high Ohnesorge and Reynolds numbers atomization occurs. |
| *Weber number* | We | $\mathrm{We} = \frac{\rho v^2 L}{\sigma}$ | Ratio of inertial forces to surface tension forces. For small Weber numbers ($\mathrm{We} \ll 1$) surface tension dominates the flow. |

Symbol definitions: $\rho$ is the fluid density, $g$ is the body force acceleration (usually the acceleration due to gravity), $L$ is the characteristic length scale for the problem, $\sigma$ is the surface tension coefficient, $\mu$ is the fluid viscosity, v is the characteristic velocity, $K^{\sigma}$ is the surface conductivity, $K^{B}$ is the bulk conductivity, $\lambda$ is the mean free path, $\alpha$ is the thermal diffusivity ($\alpha=\kappa/(\rho c_p)$), $c_p$ is the heat capacity at constant pressure, $\kappa$ is the thermal conductivity, and $T$ is the absolute temperature ($\Delta T$ is the characteristic temperature difference).

# Modeling Microfluidic Fluid Flows

This section describes the modeling of fluid flows with the Navier Stokes or Stokes equations (the section Modeling Rarefied Gas Flows gives details on how to model rarefied flows). The following topics are covered:

- Selecting the Right Physics Interface
- Single-Phase Flow
- Multiphase Flow
- Porous Media Flow
- The Relationship Between the Physics Interfaces

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- Building a COMSOL Multiphysics Model in the *COMSOL Multiphysics Reference Manual*
- Modeling Rarefied Gas Flows

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## *Selecting the Right Physics Interface*

COMSOL Multiphysics has a range of physics interfaces to use for fluid flow in a variety of circumstances. Often the selection of a particular physics interface implies certain assumptions about the equations of flow. If it is known in advance which assumptions are valid, then the appropriate physics interface can be added. However, when the flow type is unclear from the outset, or if it is difficult to reach a solution easily, starting with a simplified model and adding complexity subsequently is often a good approach. Using this approach the results of a simulation are tested against the underlying assumptions and against experimental results and the simulation can then be refined if necessary. For complex models it is often beneficial to take this approach even when the fluid flow is well characterized from the outset because a model with simplifying assumptions can be easier to solve initially. The solution process can then be fine-tuned for the more complex problem. Typically The Laminar Flow Interface is a good starting point for many problems.

The following sections describe the options available for simulating Single-Phase Flow, Multiphase Flow, and Porous Media Flow.

## *Single-Phase Flow*

The **Fluid Flow>Single-Phase Flow** branch (≋) when adding a physics interface includes the Laminar and Creeping Flow interfaces.

The Laminar Flow Interface (≋) is used primarily to model slow-moving flow in environments without sudden changes in geometry, material distribution, or temperature. The Navier-Stokes equations are solved without a turbulence model. laminar flow typically occurs at Reynolds numbers less than 1000. By default the flow is incompressible (see Figure 2-1).

The Creeping Flow Interface (≋) uses the same equations as the Laminar Flow interface with the additional assumption that the contribution of the inertia term is negligible. This is often referred to as Stokes flow and is appropriate for use when viscous flow is dominant, which is often the case in microfluidics applications. Creeping flow applies when the Reynolds number is much less than one. A creeping flow problem is significantly simpler to solve than a laminar flow problem — so it is best to make this assumption explicitly if it applies. By default the flow is incompressible (see below).

By selecting the **Neglect Inertial Form (Stokes Flow)** check-box, on the **Settings** window for **Laminar Flow** quickly convert a Laminar Flow interface into a Creeping Flow interface.

For both physics interfaces several additional options are available.

### SHALLOW CHANNEL APPROXIMATION

Often you might want to simplify long, narrow channels by modeling them in 2D. The Use Shallow Channel Approximation option is useful as it includes a drag term to approximate the added affects given by thinness of the gap between one set of boundaries in comparison to the others.

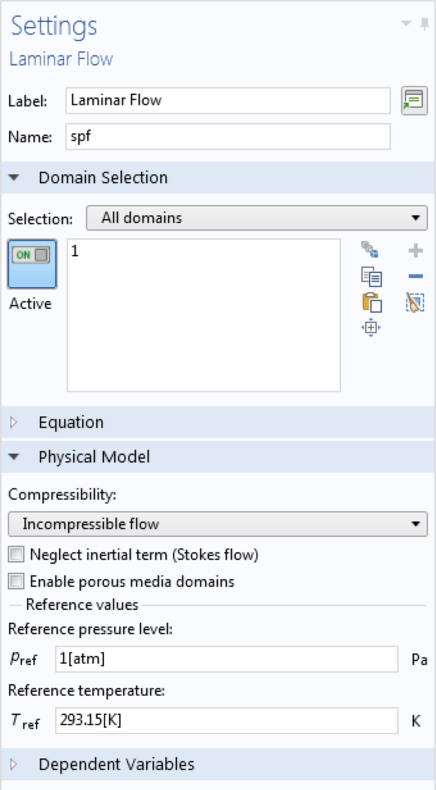
### COMPRESSIBLE FLOW

For compressible flow it is important that the density and any mass balances are well defined throughout the domain. Choosing to model incompressible flow simplifies the equations to be solved and decreases solution times. Most gas flows should be modeled as compressible flows; however, liquid flows can usually be treated as incompressible.

### NON-NEWTONIAN FLOW

The physics interfaces also allow for easy definition of non-Newtonian fluid flow through access to the dynamic viscosity in the Navier-Stokes equations. The fluid can be modeled using the power law and Carreau models or by means of any expression that describes the dynamic viscosity appropriately.

Both physics interfaces also include a feature to compute a laminar velocity profile at arbitrarily shaped inlets and outlets, which makes models much easier to set up.



Label: Laminar Flow

Name: spf

Selection: All domains

1

Compressibility: Incompressible flow

☐ Neglect inertial term (Stokes flow)

☐ Enable porous media domains

Reference pressure level:

$p_{\mathrm{ref}}$ 1[atm] Pa

Reference temperature:

$T_{\mathrm{ref}}$ 293.15[K] K

*Figure 2-1: The Settings window for Laminar Flow. Model incompressible or compressible (Ma<0.3) flow, and Stokes flow. Combinations are also possible.*

## *Multiphase Flow*

The **Multiphase Flow** branch ( ) enables the modeling of multiphase flows. These physics interfaces are included:

- The Laminar Two-Phase Flow, Level Set Interface ( ) (available under the **Two-Phase Flow, Level Set** branch ( )).
- The Laminar Two-Phase Flow, Phase Field Interface ( ) (available under the **Two-Phase Flow, Phase Field** branch ( )).
- The Laminar Two-Phase Flow, Moving Mesh Interface ( ) (available under the **Two-Phase Flow, Moving Mesh** branch ( )).

The Two-Phase Flow interfaces add surface tension forces (including the Marangoni effect) automatically at the two fluid interface(s). A library of surface tension coefficients between some common substances is available.

For problems involving topological changes (for example, jet breakup), use either the Level Set or Phase Field 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 usually produces a more accurate representation of surface tension forces, and is recommended for use in smaller scale problems with lower velocities, where the surface tension is dominant. 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).

Switch between the **Two-Phase Flow, Level Set** interface and the **Two-Phase Flow, Phase Field** interface by selecting one or other from a list available in both interfaces. This is useful if you are not sure which provides the best solution.

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 the most accurately. However, it cannot accommodate topological changes in the boundary.

For all the Two-Phase Flow interfaces, compressible flow is possible to model at speeds of less than 0.3 Mach. You can also choose to model incompressible flow by simplifying the equations to be solved. Stokes' law is also an option.

In each physics interface, the density and viscosity are specified for both fluids. You can easily use non-Newtonian models for any of the two fluids, based on the power law, the Carreau model, or using an arbitrary user-defined expression.

It is often advantageous to use more than one of these techniques to solve a problem — for example, a level set model for jet breakup could be checked prior to breakup by a moving mesh model to ensure that the surface tension is captured accurately by the diffuse interface.

---

Under the **Mathematics>Moving Interface** branch ( ) when adding an interface, The Level Set Interface ( ) and The Phase Field Interface ( ) are available in a form uncoupled with the equations of flow. These interfaces can be used to model phenomena in which other factors dominate over the fluid flow, such as some forms of phase separation.

Similarly, under the **Mathematics>Moving Mesh** branch ( ), Moving Mesh Interface ( ) is available (and described in the *COMSOL Multiphysics Reference Manual)* to treat a range of other problems involving moving meshes, such as the transport of solid particles in a fluid domain.

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## *Porous Media Flow*

The **Porous Media and Subsurface Flow** branch ( ) has the physics interfaces to model flow in porous media. The flow can be modeled by Darcy's Law or the Brinkman Equations interfaces. Additionally the Brinkman equations can be combined with laminar flow in the Free and Porous Media Flow interface.

### DARCY'S LAW

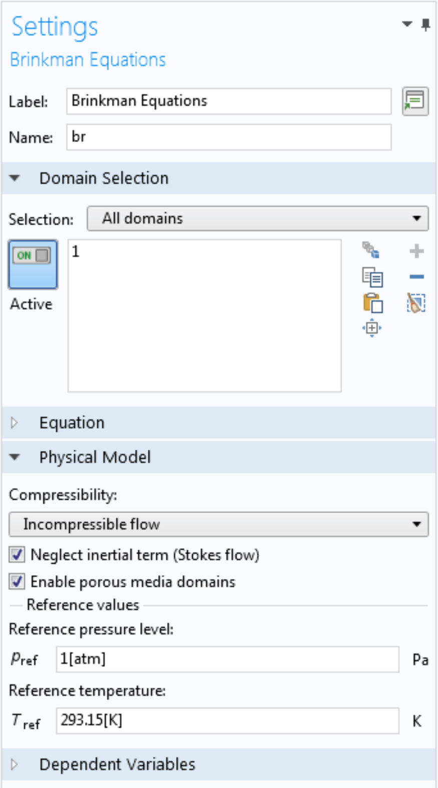
The Darcy's Law Interface ( ) is used to model fluid movement through interstices in a porous medium in the case where the fluid viscosity dominates over its inertia. Together with the continuity equation and the equation of state for the pore fluid (or gas) Darcy's law is used to model low velocity flows, for which the pressure gradient is the dominant driving force (typically when the Reynolds number of the flow is less than one). The penetration of reacting gases in a tight catalytic layer, such as a washcoat or membrane, is an example in which Darcy's law applies. Often Darcy's law is applicable for microfluidic applications, as it is appropriate for the limit of small pore size.

### BRINKMAN EQUATIONS

The Brinkman Equations Interface ( ) is used in situations where the fluid inertia, or other effects such as body forces, can no longer be neglected. Fluid penetration of filters and packed beds are applications for this physics interface. The Brinkman equations are similar in form to the Navier Stokes equations. Figure 2-2 shows the **Settings** window for the Brinkman Equations interface.

For low Reynolds number flows in which other terms in the Brinkman equations are necessary the Neglect Inertial Term (Stokes-Brinkman Flow) feature can be selected to neglect the inertial term in the equations (this is selected by default). The flow is treated as incompressible by default, but compressible flow can be enabled by selecting

**Compressible Flow (Ma<0.3)**. When using the compressible flow feature the fluid density must be defined as a function of the local pressure.



Settings

Brinkman Equations

Label: Brinkman Equations

Name: br

Domain Selection

Selection: All domains

1

Equation

Physical Model

Compressibility:

Incompressible flow

☑ Neglect inertial term (Stokes flow)

☑ Enable porous media domains

Reference values

Reference pressure level:

$p_{ref}$ 1[atm] Pa

Reference temperature:

$T_{ref}$ 293.15[K] K

Dependent Variables

*Figure 2-2: The Settings window for Brinkman Equations. Model incompressible or compressible (Ma<0.3) flow, and Stokes flow. Combinations are also possible.*

### FREE AND POROUS MEDIA

The Free and Porous Media Flow Interface ( ) has predefined couplings between the Brinkman Equations interface and the Laminar Flow interface. Porous regions of the models are included by adding a Porous Matrix Properties node with the appropriate selections to the model. The default Fluid Properties node can then be used to define regions of free laminar flow. This physics interface has all the options from both The Laminar Flow Interface and The Brinkman Equations Interface. An example application area for this physics interface would be a catalytic converter.

It should be noted that if the porous medium is large in comparison to the free channel, and the results in the region of the interface are not of interest, then it is possible to manually couple a Fluid Flow interface to the Darcy's Law interface. This makes the model computationally cheaper.

### *The Relationship Between the Physics Interfaces*

Several of the physics interfaces vary only by one or two default settings (see Table 2-4, Table 2-5) in the **Physical Model** section, which are selected either from a check box or list. For the Single-Phase Flow branch, the Laminar Flow and Creeping Flow interfaces have the same *Name* (`spf`), and this is the same for two of the Two-Phase Flow interfaces. In the Porous Media Flow branch the Free and Porous Media Flow interface combines a Laminar Flow interface with a Brinkman Equations interface (see Table 2-6).

TABLE 2-4: THE SINGLE-PHASE FLOW PHYSICAL MODEL DEFAULT SETTINGS

| PHYSICS INTERFACE LABEL | NAME | COMPRESSIBILITY | NEGLECT INERTIAL TERM (STOKES FLOW) |
|---|---|---|---|
| Laminar Flow | spf | Compressible flow (Ma<0.3) | None |
| Creeping Flow | spf | Compressible flow (Ma<0.3) | Stokes Flow |

TABLE 2-5: TWO-PHASE FLOW PHYSICAL MODEL DEFAULT SETTINGS

| PHYSICS INTERFACE LABEL | NAME | MULTIPHASE FLOW MODEL | COMPRESSIBILITY | NEGLECT INERTIAL TERM (STOKES FLOW) |
|---|---|---|---|---|
| Laminar, Two-Phase Flow, Level Set | tpf | Two phase flow, level set | Incompressible flow | None |
| Laminar, Two-Phase Flow, Phase Field | tpf | Two phase flow, phase field | Incompressible flow | None |
| Laminar, Two-Phase Flow, Moving Mesh | tpfmm | not applicable | Compressible flow (Ma<0.3) | None |

TABLE 2-6: THE POROUS MEDIA FLOW DEFAULT SETTINGS

| PHYSICS INTERFACE LABEL | NAME | COMPRESSIBILITY | NEGLECT INERTIAL TERM | PORE SIZE |
|---|---|---|---|---|
| Darcy's Law | dl | n/a | n/a | Low porosity and low permeability, slow flow |

TABLE 2-6: 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 | fp | Incompressible flow | Not selected | High permeability and porosity, fast flow |

# Modeling Coupled Phenomena in Microfluidics

In this section:

- Chemical Transport and Reactions
- Electrohydrodynamics
- Heat Transfer
- Coupling to Other Physics Interfaces

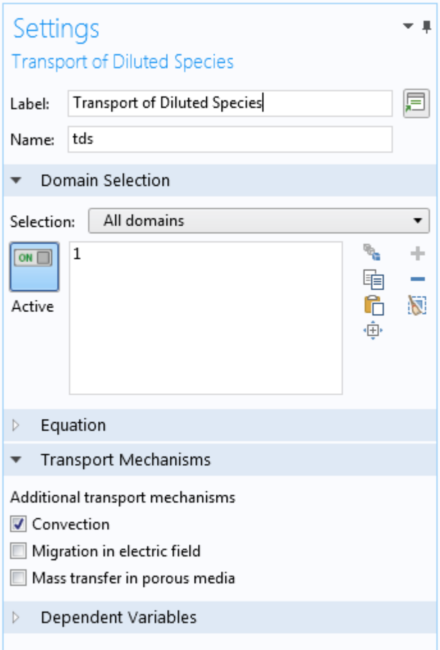
See The AC/DC Interfaces in the *COMSOL Multiphysics Reference Manual* for details, including theory, about The Electrostatics Interface and The Magnetic Fields Interface, which are included with the basic COMSOL Multiphysics license and discussed in this section.

## *Chemical Transport and Reactions*

In the Microfluidics Module, The Transport of Diluted Species Interface ( ) and The Transport of Diluted Species in Porous Media Interface ( ) are available for modeling the transport of chemical species and ions. The assumption in these physics interfaces is that one component, a solvent, is present in excess (typically more than 90 mol%). This means that the mixture properties, such as density and viscosity, are independent of concentration. To model concentrated species, the Chemical Reaction Engineering Module is recommended in addition to the Microfluidics Module.

By default the Transport of Diluted Species interface accounts for the diffusion of species by Fick's law and convection due to bulk fluid flow (see Figure 2-3). The fluid velocity field can be coupled from another physics interface (for example, Laminar Flow) by means of a domain level model input. The migration of ionic species in an electric field can also be added by selecting the appropriate check box in the Settings window for the physics interface—in this case an additional Electrostatics interface is usually coupled into the problem by an additional model input.

Chemical reactions can be added to the physics interface at the domain level by the Reactions node, which requires the Chemical Reaction Engineering Module. This allows you to specify expressions for the consumption or production of species in terms of their concentration, the concentration of other species and other model parameters, such as the temperature.



Label: Transport of Diluted Species

Name: tds

Selection: All domains

1

Additional transport mechanisms

☑ Convection

☐ Migration in electric field

☐ Mass transfer in porous media

*Figure 2-3: The Settings window for Transport of Diluted Species, with Convection selected as the Transport Mechanism by default.*

### STABILIZATION SETTINGS FOR DILUTED SPECIES TRANSPORT

For some laminar flow problems it can be useful to change the settings for the dilute species transport stabilization. To do this, click the **Show** button (  ) and select **Stabilization**. A **Consistent stabilization** section is now visible in the Transport of Diluted species settings, and in some cases it can be desirable to change the settings for the crosswind diffusion. By default the **Crosswind diffusion type** is set to **Do Carmo and Galeão**. This type of crosswind diffusion reduces undershoot and overshoot to a minimum but can in rare cases give equations systems that are difficult to fully converge. The alternative option, **Codina** is less diffusive and so should be used if the species transport is highly convective, or if convergence problems occur. This option can result in more undershoot and overshoot and is also less effective for anisotropic meshes. The Codina option activates a text field for the **Lower gradient limit** $g_{\mathrm{lim}}$ (SI unit: mol/m$^4$). It defaults to `0.1[mol/m^3)/tds.helem`, where `tds.helem` is the local element size.

For both consistent stabilization methods, the **Equation residual** can also be changed. **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 is faster to compute. If required, select **Full residual** instead.

## *Electrohydrodynamics*

*Electrohydrodynamics* is a general term describing phenomena that involve the interaction between solid surfaces, ionic solutions, and applied electric and magnetic fields. Electrohydrodynamics is frequently employed in microfluidic devices to manipulate fluids and move particles for sample handling and chemical separation.

*Electrokinetics* refers to a range of fluid flow phenomena involving electric fields. These include electroosmosis, electrothermal effects, electrophoresis and dielectrophoresis. *Electrosmosis* describes the motion of fluids induced by the forces on the charged EDLs at the surfaces of the fluid. *Electrothermal effects* occur in a conductive fluid where the temperature is modified by Joule heating from an AC electric field. This creates variations in conductivity and permittivity and thus Coulomb and dielectric body forces. *Electrophoresis* and *dielectrophoresis* describe the motion of charged and polarized particles in a non-uniform AC or DC applied field.

*Magnetohydrodynamics* refers to fluid flow phenomena involving magnetic fields. *Magnetophoresis* is the motion of diamagnetic particles in a nonuniform magnetic field and is commonly used for magnetic bead separation.

Table 2-7 summarizes these categories. Although these examples describe specific multiphysics couplings, COMSOL Multiphysics is not limited to these cases—for example, it is possible to include both magnetic and electric fields to simulate electromagnetophoresis.

TABLE 2-7: ELECTROHYDRODYNAMIC PHENOMENA

| **TYPE OF FIELD/FORCE** | **DC** | **AC** |
|---|---|---|
| **ELECTRIC FIELD (ELECTROKINETICS)** | | |
| Surface force on fluid | Electroosmosis | AC electroosmosis |
| Force on suspended particles | Electrophoresis / Dielectrophoresis | AC Electrophoresis /AC Dielectrophoresis |
| Body force on fluid | - | Electrothermal |
| Magnetic Field | | |
| Force on suspended particles | Magnetophoresis | - |

See The AC/DC Interfaces in the *COMSOL Multiphysics Reference Manual* for details, including theory, about The Electrostatics Interface and The Magnetic Fields Interface, which are included with the basic COMSOL license and discussed in this section.

### ELECTROOSMOSIS

When a polar liquid (such as water) and a solid surface (such as glass or a polymer-based substrate) come into contact, charge transfer occurs between the surface and the electrolytic solution. At finite temperature the charges on the surface are not screened perfectly by the ions in the liquid and a finite thickness *electric double layer (EDL)* or *Debye layer* develops. *Electroosmosis* is the process by which motion is induced in a liquid due to the body force acting on the EDL in an electric field.

A complete model of the system includes the space charge layer explicitly. The electric potential is the solution of a nonlinear partial differential equation, the Poisson-Boltzmann equation, which can be solved by coupling an Electrostatics interface to a Transport of Diluted Species interface (with migration enabled) for the ion species. The software then computes the forces on the fluid and a further coupled Laminar Flow or Creeping Flow interface is used to compute the overall fluid flow. In practice this approach is only possible for nanoscale channels—as typically the EDL thickness is 1-10 nm.

The Poisson Boltzmann equation is sometimes linearized—this is referred to as the Debye-Hückel approximation which applies when $ze\zeta \ll k_B T$, where $\zeta$ is the potential at the surface of the moving volume of fluid (the *zeta potential*). At room temperature this corresponds to the limit $\zeta \ll 26$ mV. Note that there is a layer of immobile ions trapped adjacent to the surface (the *Stern Layer*, which is of order one hydrated ion radius thick) with an associated volume of immobile fluid; this means that $\zeta$ is not simply the wall potential. $\zeta$ is usually determined experimentally from electroosmotic flow measurements.

The Poisson-Boltzmann equation has a characteristic length scale—the Debye length, $\lambda_D$:

$$\lambda_D = \sqrt{\frac{\varepsilon k_B T}{2z^2e^2c_\infty}}$$

where $k_B$ is Boltzmann's constant, $T$ is the temperature, $z$ is the ion's valance number, $e$ is the electron charge, and $c_\infty$ is the ion's molar concentration in the bulk solution. When the Debye length is small compared to the channel thickness, the electroosmotic flow velocity can be modeled by the *Helmholtz-Smoluchowski equation*:

$$u_{\mathrm{eo}} = \frac{\varepsilon\zeta}{\mu}E$$

where $E$ is the applied electric field and $\mu$ is the liquid's dynamic viscosity. From this equation, the electroosmotic mobility is naturally defined as:

$$\mu_{\mathrm{eo}} = \frac{\varepsilon\zeta}{\mu} \tag{2-1}$$

The Laminar Flow and Creeping Flow interfaces include a wall boundary condition option for an Electroosmotic Velocity boundary condition. This enables you to specify the external electric field (which can be manually specified or coupled from an Electrostatics interface) and the electroosmotic mobility to define an electroosmotic flow.

Further details of the theory of electroosmosis can be found in Ref. 1 and Ref. 2.

### AC ELECTROOSMOSIS

Because an alternating electric field does not generate a net force on the EDL, AC electroosmosis is not used for fluid transport in microfluidics. However, the back-and-forth movements an AC field generates are useful for mixing purposes. To model AC electroosmotic flow when the frequency of the electric field is sufficiently low, the same approaches can be taken as for DC electroosmosis. An Electrostatics interface should still be employed to calculate the electric field, but when this is coupled into other physics interfaces the AC dependence should be explicitly added using an expression. With increasing frequency, AC electroosmosis becomes less important so this approach is valid for most practical examples.

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*Electro-osmotic Micromixer*: Application Library path **Microfluidics_Module/Micromixers/electroosmotic_mixer**

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### ELECTROPHORESIS

Electrophoresis describes the motion of charged particles or molecules suspended in a liquid due to an applied electric field.

In COMSOL Multiphysics it is easy to calculate the electrophoretic velocity for spherical particles for the cases when the Debye length is much smaller or much larger than the particle size. If the surface conductivity of the particle can be neglected (this is sometimes referred to as the limit or small Dukhin number) the electrophoretic velocity (the particle velocity relative to the bulk flow) is given by:

$$\mathbf{u}_{\mathrm{ep}} = \frac{2}{3}\mu_{\mathrm{eo}} f\left(\frac{a}{\lambda_D}\right)\mathbf{E}$$

where a is the radius of the particle, $\mathbf{E}$ is the electric field, and $f(a/\lambda_{\mathrm{D}})$ is known as Henry's function (note that $f(a/\lambda_D)$ is often written as $f(\kappa a)$ where $\kappa = 1/\lambda_D$). Henry's function takes the value of 1 in the limiting case where $a \ll \lambda_D$ (often known as the Hückel approximation) and 3/2 in the case where $a \gg \lambda_D$ (this is equivalent to Equation 2-1 and is referred to as the Smoluchowski approximation). Note that if $\lambda_D$ is large compared to the fluid volume, the charge is effectively unscreened and the electric force is simply that due to the charge on the molecule. The following result is obtained from the force balance between the Stokes drag and the electric force for an unscreened charged particle:

$$\mathbf{u}_{\mathrm{ep}} = \frac{q}{6\pi\mu a}\mathbf{E}$$

where $q$ is the charge on the molecule and $\mu$ is the fluid viscosity. Further details of the theory of electroosmosis can be found in Ref. 2.

These velocity fields can be computed directly from an electric field calculated by the Electrostatics interface. If necessary the velocity can be added to the flow velocity field to compute the net particle velocity.

## DIELECTROPHORESIS

*Dielectrophoresis* (DEP) describes the motion of polarizable particles suspended in a fluid with an applied nonuniform electric field. The electric field induces a dipole moment on the particles, which in turn produces a net force. In the following discussion the general case of AC electrophoresis is treated, which is more commonly used for practical reasons (see Ref. 1 for further details).

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For a DC field these results can be applied if $\mathbf{E}_{\mathrm{rms}}=\mathbf{E}$ is used.

---

The time-dependent dielectrophoretic force acting on a particle in an applied field is given by (Ref. 1):

$$\mathbf{F}_{\mathrm{DEP}}(t) = 2\pi\varepsilon_m a^3 K(\varepsilon_m,\varepsilon_p)\nabla(\mathbf{E}(t)\cdot\mathbf{E}(t)) \qquad (2\text{-}2)$$

where $\varepsilon_m$ and $\varepsilon_p$ are the complex permittivities of the medium and the particle respectively, $a$ is the radius of the particle's equivalent homogeneous sphere and $K(\varepsilon_m,\varepsilon_p)$ is the Clausius-Mossotti function. The complex permittivity, $\varepsilon^*$, for an isotropic homogeneous dielectric is

$$\varepsilon^* = \varepsilon - i\frac{\sigma}{\omega}$$

where $\varepsilon$ is the electric permittivity, $\sigma$ is the electrical conductivity, and $\omega$ is the angular field frequency. The Clausius-Mossotti function is given by:

$$K(\varepsilon_m, \varepsilon_p) = \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m}$$

which depends on the particle's complex permittivity, $\varepsilon_p$, and that of the medium, $\varepsilon_m$.

Taking the time average of Equation 2-2 gives the time averaged force:

$$\langle\mathbf{F}_{\mathrm{DEP}}(t)\rangle = 2\pi\varepsilon_m r_0 \mathrm{Re}(K(\varepsilon_m, \varepsilon_p))\nabla(\mathbf{E}_{\mathrm{rms}}\cdot\mathbf{E}_{\mathrm{rms}})$$

By balancing this force with the Stokes drag force the dielectrophoretic velocity is obtained:

$$\mathbf{u}_{\mathrm{DEP}} = \frac{\varepsilon_m r_0 \mathrm{Re}(K(\varepsilon_m, \varepsilon_p))\nabla(\mathbf{E}_{\mathrm{rms}}\cdot\mathbf{E}_{\mathrm{rms}})}{3\mu}$$

where μ is the dynamic viscosity.

The value of $\mathbf{E}_{\mathrm{rms}}$ can be computed from an Electrostatics interface in which the root mean square (RMS) voltages are applied as boundary conditions. The gradient of the field can then be computed term by term from the spatial derivatives of an expression for the dot product of the electric field with itself. Finally the dielectrophoretic velocity term can be added to the velocity field to compute the particle velocity field.

### MAGNETOPHORESIS

Particles with an induced or permanent magnetization can be moved relative to a fluid flow by the application of an external, inhomogeneous magnetic field. This process is analogous to dielectrophoresis and is usually termed magnetophoresis. In the case of a nonconducting particle, in a static, irrotational external applied field, $\mathbf{H}_{\mathrm{ext}}$, the magnetophoretic force is given by (Ref. 1):

$$\mathbf{F}_{MAP} = 2\pi\mu_m K(\mu_m, \mu_p) a^3 \nabla(\mathbf{H}_{\mathrm{ext}} \cdot \mathbf{H}_{\mathrm{ext}})$$

where $\mu_m$ and $\mu_p$ are the permeabilities of the medium and the particle respectively (usually $\mu_m = \mu_0$), $a$ is the radius of the particle's equivalent homogeneous sphere and $K(\mu_m, \mu_p)$ is the Clausius-Mossotti function. Note that the external magnetic field, $\mathbf{H}_{ext}$, should be distinguished from the local field **H** which includes contributions from the particle itself. In this case the Clausius-Mossotti function is given by:

$$K(\mu_m, \mu_p) = \frac{\mu_p - \mu_m}{\mu_p + 2\mu_m}$$

By balancing this force with the Stokes drag force the magnetophoretic velocity is obtained:

$$\mathbf{u}_{MAP} = \frac{\mu_m r_0 K(\mu_m, \mu_p) \nabla(\mathbf{H}_{ext} \cdot \mathbf{H}_{ext})}{3\mu}$$

where μ is the dynamic viscosity.

The value of $\mathbf{H}_{\mathrm{ext}}$ can be computed from a Magnetic Fields or a Magnetic Fields, No Currents interface.

> The Magnetic Fields, No Currents interface requires the AC/DC Module.

The Magnetic Fields Interface in the *COMSOL Multiphysics Reference Manual*

The gradient of the field can then be computed term by term from the spatial derivatives of an expression for the dot product of the magnetic field with itself. Finally the magnetophoretic velocity term can be added to the velocity field to compute the particle velocity field.

### ELECTROTHERMALLY-DRIVEN FLOW

Electrothermal body forces arise from electrically generated, nonuniform Joule heating, which creates variations in conductivity and permittivity and thus Coulomb and dielectric body forces. It is possible to determine the resulting fluid motion by solving the Navier-Stokes equations with an additional electrothermal body force term. The electric field is once again assumed to be quasi-static and can be coupled in from an Electrostatics interface.

The electrothermal force is given by:

$$\mathbf{F} = -\frac{1}{2}\left[\left(\frac{\nabla\sigma}{\sigma}+\frac{\nabla\varepsilon}{\varepsilon}\right)\cdot\mathbf{E}\frac{\varepsilon\mathbf{E}}{1+(\omega\tau)^2}+\frac{1}{2}|\mathbf{E}|^2\nabla\varepsilon\right]$$

where $\sigma$ is the conductivity, $\varepsilon$ is the fluid's permittivity, $\omega$ is the angular frequency of the electric field, and $\tau = \varepsilon/\sigma$ is the fluid's charge-relaxation time. The electric-field vector $\mathbf{E}$ contains the amplitude and direction of the AC electric field but not its instantaneous value.

Because of the heating, $\varepsilon$ and $\sigma$ are temperature dependent, and their gradients are functions of the temperature gradient: $\nabla\varepsilon = (\partial\varepsilon/\partial T)\nabla T$ and $\nabla\sigma = (\partial\sigma/\partial T)\nabla T$. With water, for example, the relative change rates for the permittivity and the conductivity are $(1/\varepsilon)(\partial\varepsilon/\partial T) = -0.004\ 1/\mathrm{K}$ and $(1/\sigma)(\partial\sigma/\partial T) = 0.02\ 1/\mathrm{K}$, respectively.

### ELECTROWETTING

The contact angle of a two-fluid interface with a solid surface is determined by the balance of the forces at the contact point. The equilibrium contact angle, $\theta_0$, is given by Young's equation:

$$\gamma_{s1}+\sigma_{12}\cos\theta_0 = \gamma_{s2}$$

Here $\gamma_{s1}$ is the surface energy per unit area between fluid 1 and the solid surface, $\gamma_{s2}$ is the surface energy per unit area between fluid 2 and the solid surface, and $\sigma_{12}$ is the surface tension at the interface between the two fluids.

In *electrowetting* the balance of forces at the contact point is modified by the application of a voltage between a conducting fluid and the solid surface. For many applications the solid surface consists of a thin dielectric deposited onto a conducting layer; this is often referred to as *Electrowetting on Dielectric* (EWOD). In this case, the capacitance of the dielectric layer dominates over the double layer capacitance at the solid-liquid interface (Ref. 3). The energy stored in the capacitor formed between the conducting liquid and the conducting layer in the solid reduces the effective surface energy of the liquid to which the voltage is applied. For the case when a voltage difference occurs between fluid 1 and the conductor beyond the dielectric Young's equation is modified as follows:

$$\gamma_{s1} - \frac{\varepsilon V^2}{2d_f} + \sigma_{12}\cos\theta_{\mathrm{ew}} = \gamma_{s2}$$

Here $\varepsilon$ is the permittivity of the dielectric, $V$ is the potential difference applied, and $d_f$ is the dielectric thickness. This equation can be rewritten as

$$\cos\theta_{\mathrm{ew}} = \cos\theta_0 + \frac{\varepsilon V^2}{2\sigma_{12}d_f} \qquad (2\text{-}3)$$

Electrowetting can therefore be used to modify the contact angle dynamically by changing the applied voltage.

The EWOD applications can be modeled by using Equation 2-3 as an expression for the contact angle. This can simply be entered as the value of the contact angle in the Two-Phase Flow interface that is being used. Note that the software automatically handles a time varying voltage in this expression.

For step-by-step instructions, see *Electrowetting Lens*: Application Library path **Microfluidics_Module/Two-Phase_Flow/electrowetting_lens**.

## *Heat Transfer*

It is often necessary to consider the effect of heat flow and temperature dependent material properties (such as the viscosity or the surface tension) in microfluidic systems. The COMSOL Multiphysics base package includes physics interfaces for heat transfer in incompressible fluids and solids. The Heat Transfer Module is required in addition to this module to model heat flow in compressible fluids and to include viscous heating terms. This section describes how to couple heat transfer to microfluidics models using the functionality available in the COMSOL Multiphysics base package and the Microfluidics Module.

The Heat Transfer interface includes the equations for heat transfer in both fluid and solid domains. To model a system consisting of both solid and liquid domains add a single Heat Transfer interface and then add nodes for Heat Transfer in Solids and Heat Transfer in Fluids with selections corresponding to the solid and fluid domains respectively. For a fluid domain the convective flow is coupled into domain by selecting the velocity field from a corresponding Laminar Flow or Creeping Flow interface.

The fluid domain models the heat transfer including both convection and conduction according to the equation:

$$\rho C_p\left(\frac{\partial T}{\partial t} + (\mathbf{u}\cdot\nabla)T\right) = -(\nabla\cdot\mathbf{q}) + Q$$

where, $\rho$ is the fluid density (SI unit: kg/m$^3$), $C_\mathrm{p}$ is the specific heat capacity at constant pressure (SI unit: J/(kg·K)), $T$ is absolute temperature (SI unit: K), $\mathbf{u}$ is the velocity vector (SI unit: m/s), $\mathbf{q}$ is the heat flux by conduction (SI unit: W/m$^2$), and $Q$ contains heat sources other than viscous heating (SI unit: W/m$^3$). For a solid domain the following equation applies:

$$\rho C_p\frac{\partial T}{\partial t} = -(\nabla\cdot\mathbf{q}) + Q$$

When using the heat transfer in solids and in fluids domain properties the software automatically includes the heat transfer between the solid and the fluid. It is important to include the correct thermal boundary conditions on regions where fluid flows into or out of a domain, typically a Temperature condition for an inlet and an Outflow condition for an outlet.

For a detailed discussion of the fundamentals of heat transfer, see Ref. 4. More details of the heat transfer capabilities can be found in The Heat Transfer Interfaces in the *COMSOL Multiphysics Reference Manual*.

## *Coupling to Other Physics Interfaces*

COMSOL is not limited to the common couplings described in this chapter—there are many other phenomena that can be easily modeled in microfluidics. In many cases physics interfaces can be coupled simply by entering expressions from one physics interface (such as the local temperature) into fields in another physics interface (for example in the **Model Inputs** section of a **Fluid Properties** node). Additionally COMSOL includes powerful coupling operators that enable physics interfaces to be linked by projections, extrusions, or scalar quantities such as integrals and global averages.

Component Couplings and Coupling Operators in the *COMSOL Multiphysics Reference Manual*

# Modeling Rarefied Gas Flows

In this section:

- The Flow Regimes
- Slip Flow
- References for the Theory of Microfluidics

## *The Flow Regimes*

Rarefied gas flow occurs when the mean free path, $\lambda$, of the molecules becomes comparable with the length scale of the flow, $l$. There are four flow regimes depending on the value of the Knudsen number, $Kn=\lambda/l$ (Ref. 5):

- Continuum flow ($\mathrm{Kn}<0.01$)
- Slip flow ($0.01<\mathrm{Kn}<0.1$)
- Transitional flow ($0.1<\mathrm{Kn}<10$)
- Free molecular flow ($\mathrm{Kn}>10$)

These flow regimes are shown in Figure 2-4. In the ***continuum flow*** regime the Navier-Stokes equations are applicable, as discussed in Modeling Microfluidic Fluid Flows. Gases flowing in the slip flow regime can be modeled using the Navier-Stokes equations with modified boundary conditions. The Slip Flow interface is included with the Microfluidics Module and can be used to model gas flows at these moderate Knudsen numbers. The Molecular Flow Module includes the Transitional Flow and the Free Molecular Flow interfaces, which can be used to model fully kinetic gas flows, at Knudsen numbers greater than 0.1.

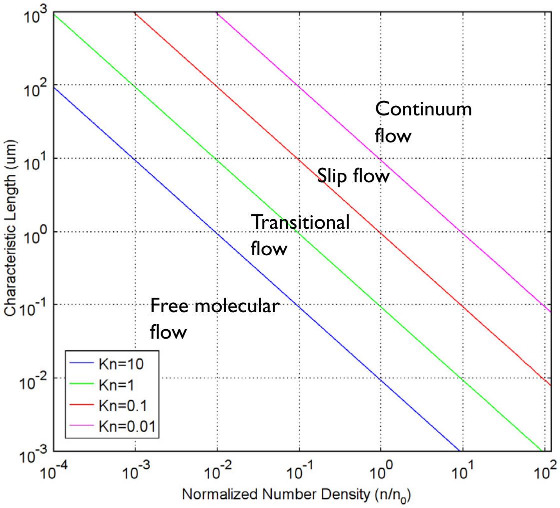

*Figure 2-4: A plot showing the main fluid flow regimes for rarefied gas flows. Different regimes are separated by lines of constant Knudsen numbers. The number density of the gas is normalized to the number density of an ideal gas at a pressure of 1 atmosphere and a temperature of 0° C ($n_0$).*

## *Slip Flow*

In the slip flow regime, the Navier-Stokes equations can still be used with modified boundary conditions to account for rarefaction effects close to the wall. A layer of rarefied gas with a size similar to the mean free path develops close to the wall—this is termed the *Knudsen layer*. The Navier-Stokes equations are not applicable in this layer, but the flow outside the layer can be described by extrapolating the bulk gas flow toward the wall and applying Maxwell's slip boundary condition at the wall (Ref. 5). For thermal flows the von Smoluchowski temperature jump boundary condition must also be applied (Ref. 5).

To model flows in the slip flow regime use the Slip Flow interface. That physics interface can be used to model isothermal and non-isothermal flows with or without explicit modeling of thermal processes in adjacent solid domains. To model isothermal flows use the Temperature boundary condition on all external model surfaces, with the temperature set equal to the fluid temperature. The Slip Wall and External Slip Wall boundary conditions are used to model slip on interior and exterior model boundaries respectively. These boundary conditions include thermal creep or transpiration, viscous slip, and the von Smoluchowski temperature jump. The slip coefficients can be specified directly or by means of Maxwell's model. For further details see The Slip Flow Interface and Theory for the Slip Flow Interface.

- The Temperature boundary condition is described for the Heat Transfer interface in the *COMSOL Multiphysics Reference Manual*.
- Slip Velocity

## *References for the Theory of Microfluidics*

1. H. Bruus, *Theoretical Microfluidics*, Oxford University Press, 2008.

2. R.F. Probstein, *Physicochemical Hydrodynamics: An Introduction*, 2nd ed., Wiley-Interscience, 2003.

3. F. Mugele and J.C. Baret, "Electrowetting: from basics to applications," *J. Phys. Condens. Matter*, vol. 17, pp. R705–R774, 2005.

4. F.P. Incropera and D.P. DeWitt, *Fundamentals of Heat and Mass Transfer*, 4th ed., John Wiley & Sons, 1996.

5. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

# 3

# Single-Phase Flow Interfaces

There are several Fluid Flow interfaces available with the Microfluidics Module. These are grouped by type and found under the **Fluid Flow>Single-Phase Flow** branch (≋) when adding a physics interface. See Modeling Microfluidic Fluid Flows to help you select which physics interface to use.

In this chapter:

- The Laminar Flow and Creeping Flow Interfaces
- Theory for the Single-Phase Flow Interfaces

# The Laminar Flow and Creeping Flow Interfaces

In this section:

- The Creeping Flow Interface
- The Laminar Flow 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 2-3 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings** sections, 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.

## *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)** check box is selected. If unchecked, 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.

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

### CONSISTENT STABILIZATION

This check box is selected by default and should remain selected for optimal performance. The consistent stabilization method does not perturb the original transport equation.

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

- *Transport in an Electrokinetic Valve*: Application Library path **Microfluidics_Module/Fluid_Flow/electrokinetic_valve**
- *Controlled Diffusion Micromixer*: Application Library path **Microfluidics_Module/Micromixers/controlled_diffusion_micromixer**

## *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 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 re-set 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.

If the **Neglect inertial term (Stokes flow)** check box 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** and at the **Reference temperature** defined in **Reference values**. The fluid dynamic viscosity is evaluated at the **Reference temperature**.

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 **Reference values**.

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.

### *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** check box 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.

### *Use Shallow Channel Approximation*

For 2D components, selecting the **Use shallow channel approximation** check box 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 $\mu$ 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 and viscosity of the fluid when the **Incompressible flow** or the **Weakly compressible flow** option is selected.

**Reference pressure level** There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A=p+p_{\mathrm{ref}}$, or the gauge pressure $p$. When $p_{\mathrm{ref}}$ 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 .

**Reference temperature** The reference temperature is .

**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.**

## 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 may 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.

## ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. 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.

- Pseudo Time Stepping for Laminar Flow Models
- Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow
- Theory for the Single-Phase Flow Interfaces

### 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 these can 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 since 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**

## *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
- Flow Continuity
- Fluid Properties
- Initial Values
- Inlet
- Line Mass Source[1]
- Open Boundary
- Outlet
- Periodic Flow Condition
- Pipe Connection[1]
- Point Mass Source[1]
- Pressure Point Constraint
- Symmetry
- Volume Force
- Wall

[1] A feature that may require an additional license

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 2-3 for links to common sections and Table 2-4 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 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.

### 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. If a Heat Transfer interface is included in the component, the temperature field 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 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 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 $p$+$p_{\mathrm{ref}}$, where $p$ is the dependent pressure variable from the Navier-Stokes or RANS equations, and $p_{\mathrm{ref}}$ is from the user input defined at the physics interface level. When $p_{\mathrm{ref}}$ is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, $p_{\mathrm{ref}}$ 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

### *Density*

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible (at the physics interface level).

### Dynamic Viscosity

The **Dynamic viscosity** $\mu$ 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.

Using the built-in variable for the shear rate magnitude, `spf.sr`, makes it possible to define arbitrary expressions of the dynamic viscosity as a function of the shear rate.

For laminar flow, the **Non-Newtonian power law** may be used to model the viscosity of a non-Newtonian fluid. The following model parameters are required for the **Non-Newtonian power law**:

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

Alternatively, the **Non-Newtonian Carreau model** may be used to model the viscosity of a non-Newtonian fluid for laminar flow. The following Carreau model parameters are required:

- **Zero shear rate viscosity** $\mu_0$
- **Infinite shear rate viscosity** $\mu_{\mathrm{inf}}$
- **Model parameter** $\lambda$ and $n$

The non-Newtonian fluids models have a shear-rate dependent viscosity. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions. See Non-Newtonian Flow: The Power Law and the Carreau Model in the *CFD Module User's Guide*.

## 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** $p$.

## *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
- Slip
- Electroosmotic Velocity
- Slip Velocity
- Leaking Wall

#### *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 $\mathbf{u} = 0$.

#### *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.

#### *Electroosmotic Velocity*

When an electric field drives a flow along the boundary, the components for the **Electric field** $\mathbf{E}$ along with the **Electroosmotic mobility** $\mu_{eo}$ should be defined. The **Built-in**

**expression** for the **Electroosmotic mobility** requires values or expressions for the **Zeta potential** $\zeta$ and the **Relative permittivity** $\varepsilon_r$.

### *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** check box 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** $\lambda$ 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** check box is selected, a thermal creep contribution with **Thermal slip coefficient** $\sigma_T$ 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.

### *Navier Slip*

This boundary condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{\mathrm{wall}} = 0$ and adds a frictional force of the form

$$\mathbf{F}_{\mathrm{fr}} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\beta$ is a slip length. The slip length is defined as $\beta = h_{\mathrm{min}}/2$, where $h_{\mathrm{min}}$ is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements). The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance $\beta$ outside of the wall.

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

### *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.

### 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** $\mathbf{u}_{\mathrm{w}}$ 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** $U_{\mathrm{w}}$ should be specified in 2D.

### CONSTRAINT SETTINGS

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

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

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## *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, Laminar inflow**, **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 $\mathbf{u} = -\mathbf{n}\mathrm{U}_0$, 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.

### PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure. If the reference pressure $p_{\mathrm{ref}}$, 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.

- The **Suppress backflow** option adjusts the inlet pressure locally in order to prevent fluid from 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** $\mathbf{d}_{\mathbf{u}}$ (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.

### LAMINAR INFLOW

This boundary condition is applicable when the fluid enters the domain from a long pipe or channel, in which the laminar flow profile is fully developed. The normal stress at the inlet is determined from the flow conditions at the entrance to a fictitious channel of length $L_{\mathrm{entr}}$ appended to the boundary. The inflow can be specified by the **Average velocity** $U_{\mathrm{av}}$, the **Flow rate** $V_0$, or the **Entrance pressure** $p_{\mathrm{entr}}$.

the **Entrance pressure** $p_{\mathrm{entr}}$ The **Entrance length** $L_{\mathrm{entr}}$ should be significantly greater than $0.06\mathrm{Re}D$, where Re is the Reynolds number and $D$ is the inlet length scale (hydraulic diameter), in order that the flow can adjust to a fully developed laminar profile.

The **Constrain outer edges to zero** option forces the laminar profile to go to zero at the bounding points or edges of the inlet channel. Otherwise the velocity is defined by the boundary condition of the adjacent boundary in the computational domain. For example, if one end of a boundary with a **Laminar inflow** condition connects to a slip boundary, the laminar profile will have a maximum at that end.

### 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)**.

#### *Mass Flow Rate*

The **Mass flow rate** option sets the integrated mass flow across the entire boundary, 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** $d_{\mathrm{bc}}$ 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** $Q_{\mathrm{sv}}$ 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** $V_{\mathrm{m}}$ (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** $V_{\mathrm{m}}$ should be specified.
- **Standard pressure and temperature**, for which the **Standard pressure** $P_{\mathrm{st}}$ and the **Standard temperature** $T_{\mathrm{st}}$ should be defined.

For 2D components, the **Channel thickness** $d_{\mathrm{bc}}$ 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** $Q_{\mathrm{sccm}}$ should be specified.

-

### 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

## *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, Laminar outflow**, and **Velocity**.

### 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. If the reference pressure $p_{\mathrm{ref}}$, 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.

- 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** check box is selected by default. This option adjusts the outlet pressure in order to prevent fluid from entering the domain through the boundary.

### VELOCITY

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

### LAMINAR OUTFLOW

This boundary condition is applicable when the flow exits the domain into a long pipe or channel, at the end of which a laminar flow profile is fully developed. The normal stress at the outlet is determined from the flow conditions at the end of a fictitious channel appended to the outlet boundary. The outflow can be specified by the **Average velocity** $U_{\mathrm{av}}$, the **Flow rate** $V_0$, or the **Exit pressure** $p_{\mathrm{exit}}$.

The **Exit length** $L_{\text{exit}}$ should be significantly greater than 0.06Re$D$, where Re is the Reynolds number, and $D$ is the outlet length scale (hydraulic diameter), in order that the flow can adjust to a fully developed laminar profile.

The **Constrain outer edges to zero** option forces the laminar profile to go to zero at the bounding points or edges of the outlet channel. Otherwise, the velocity is defined by the boundary condition of the adjacent boundary in the computational domain. For example, if one end of a boundary with a **Laminar outflow** condition connects to a slip boundary, the laminar profile will have a maximum at that end.

#### CONSTRAINT SETTINGS

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

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Prescribing Inlet and Outlet Conditions

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## *Symmetry*

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:

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

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

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:

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

#### 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 $p \approx f_0$ .

#### 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.

## *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 $\mathbf{F}$:

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

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

for the compressible and the incompressible formulations.

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

$$p = 2\mu\frac{\partial u_n}{\partial n}-\mathbf{n}\cdot\mathbf{F} \qquad (3\text{-}2)$$

If $\partial u_n/\partial n$ is small, Equation 3-2 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:

$$\mathbf{n}^T\left(-p\mathbf{I}+\left(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = -\mathrm{f}_0, \qquad \mathbf{t}\cdot\mathbf{u} = 0$$

$$\mathbf{n}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -\mathrm{f}_0, \qquad \mathbf{t}\cdot\mathbf{u} = 0$$

for the compressible and the incompressible formulations.

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

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

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

#### 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.

## *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, it is recommended to only include two boundaries.

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.

#### PRESSURE DIFFERENCE

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

A value or expression should be specified for the **Pressure difference**, $p_{\mathrm{src}} - p_{\mathrm{dst}}$. 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** 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*.

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## Pipe Connection

This feature is available with a license for the Pipe Flow Module. For details, see Pipe Connection the in the *Pipe Flow Module User's Guide*.

## 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.

A Wall 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 **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Flow Continuity** node, additional Fallback feature subnodes can be added.

- Turbulent Flow, Algebraic yPlus

### STUDY

The **Study** section contains two down-list: **Study type** and **Initial value from study**. The when Turbulence flow, k-ε or Turbulence flow, k-ω is selected, the **Study type** contains two options:

- Stationary
- Time-dependent

The default value is **Stationary**. Otherwise, the **Study type** contains two options:

- Stationary with initialization
- Transient with initialization

The default value is **Stationary with initialization**. Note that the created new study only solve for the new turbulence model.

**Initial value from study** contains a list of available study and **None**. If there is no study available, the default option is **None**. If there are available studies, the first study will be the default option.

## *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** $p_0$. Or, if the reference pressure $p_{\mathrm{ref}}$ defined at the physics interface level is equal to zero, $p_0$ represents the absolute pressure.

### CONSTRAINT SETTINGS

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

## *Point Mass Source*

This feature requires at least one of the following licenses: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition 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 Batteries & Fuel Cells 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**, $\dot{q}_{\mathrm{p}}$ 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: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition 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 Batteries & Fuel Cells 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**, $\dot{q}_l$, 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*

## *Gravity*

This feature requires at least one of the following licenses: CFD Module, Heat Transfer Module.

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.

### ACCELERATION OF GRAVITY

The **Acceleration of gravity** (SI unit m/s, default value $-g_{\mathrm{const}}\mathbf{e}_\mathbf{z}$ in 2Daxi and 3D and $-g_{\mathrm{const}}\mathbf{e}_\mathbf{y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

# Theory for the Single-Phase Flow 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: The Power Law and the Carreau Model
- Gravity
- The Boussinesq Approximation
- Theory for the Wall Boundary Condition
- Prescribing Inlet and Outlet Conditions
- Laminar Inflow
- Laminar Outflow
- Mass Flow
- No Viscous Stress
- Normal Stress Boundary Condition
- Mass Sources for Fluid Flow
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- Discontinuous Galerkin Formulation

- 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

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0 \tag{3-4}$$

$$\rho\frac{\partial\mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \tau] + \mathbf{F} \tag{3-5}$$

$$\rho C_p\left(\frac{\partial T}{\partial t} + (\mathbf{u}\cdot\nabla)T\right) = -(\nabla\cdot\mathbf{q}) + \tau{:}\mathbf{S} - \frac{T}{\rho}\frac{\partial\rho}{\partial T}\bigg|_p\left(\frac{\partial p}{\partial t} + (\mathbf{u}\cdot\nabla)p\right) + Q \tag{3-6}$$

where

- $\rho$ 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)
- $\tau$ is the viscous stress tensor (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: $\mathrm{N/m^3}$)
- $C_\mathrm{p}$ 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:

$$\mathbf{S} = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

The operation “:” denotes a contraction between tensors defined by

$$\mathbf{a}:\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm} \tag{3-7}$$

This is sometimes referred to as the double dot product.

Equation 3-4 is the continuity equation and represents conservation of mass. Equation 3-5 is a vector equation which represents conservation of momentum. Equation 3-6 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 3-4 through Equation 3-6, constitutive relations are needed. For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

$$\tau = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I} \tag{3-8}$$

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. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions. With the Microfluidics Module, you can model flows of non-Newtonian fluids using the predefined power law and Carreau models, which describe the dynamic viscosity for non-Newtonian fluids.The Heat Transfer Module treats all fluids as Newtonian according to Equation 3-8.Other commonly used constitutive relations are Fourier's law of heat conduction and the ideal gas law.

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 3-6 is decoupled from Equation 3-4 and Equation 3-5.

### 2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 3-4 and Equation 3-5 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 $\phi$ -equation can be removed from Equation 3-5. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the $\phi$ -equation. The default 2D axisymmetric formulation of Equation 3-4 and Equation 3-5 therefore assumes that

$$\partial/\partial\phi = 0$$
$$u_\phi = 0$$

## Compressible Flow

The equations of motion for a single-phase fluid are the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0 \tag{3-9}$$

and the momentum equation:

$$\rho\frac{\partial\mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nabla\cdot\left(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right) + \mathbf{F} \tag{3-10}$$

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.

## 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 3-10, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 3-9, 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 3-10 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.

The practical Mach number limit is lower than one, however. 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.

## *Incompressible Flow*

When the temperature variations in the flow are small, a single-phase fluid can often be assumed incompressible; that is, $\rho$ 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 3-9 reduces to

$$\rho\nabla\cdot\mathbf{u} = 0 \tag{3-11}$$

and Equation 3-10 becomes

$$\rho\frac{\partial\mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F} \tag{3-12}$$

In order to apply the incompressible flow formulation, the density is evaluated at the reference pressure level, and both the density and viscosity are evaluated at the reference temperature. However, if the density is a function of other quantities such as a concentration field, 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:

$$\mathrm{Re}=\frac{\rho UL}{\mu}$$

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.

Observe 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 $\mathrm{Re}^c$ grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as: `spf.cellRe`).

## *Non-Newtonian Flow: The Power Law and the Carreau Model*

The viscous stress tensor is directly dependent on the shear rate tensor and can be written as:

$$\tau = \mu\dot{\boldsymbol{\gamma}} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$$

$$\tau = \mu\dot{\boldsymbol{\gamma}}$$

using the compressible and incompressible formulations. Here $\dot{\boldsymbol{\gamma}}$ denotes the strain-rate tensor defined by:

$$\dot{\boldsymbol{\gamma}} = (\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

Its magnitude, the shear rate, is:

$$\dot{\gamma} = |\dot{\boldsymbol{\gamma}}| = \sqrt{\frac{1}{2}\dot{\boldsymbol{\gamma}}:\dot{\boldsymbol{\gamma}}}$$

where the contraction operator ":" is defined by

$$\mathbf{a}:\mathbf{b} = \sum_n \sum_m a_{nm} b_{nm}$$

For a *non-Newtonian fluid*, the dynamic viscosity is assumed to be a function of the shear rate:

$$\mu = \mu(\dot{\gamma})$$

The Laminar Flow interfaces have the following predefined models to prescribe a non-Newtonian viscosity—the power law and the Carreau model.

### POWER LAW

The power law model is an example of a generalized Newtonian model. It prescribes

$$\mu = m\dot{\gamma}^{n-1} \tag{3-13}$$

where $m$ and $n$ are scalars that can be set to arbitrary values. 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 3-13 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 $10^{-2}\ \mathrm{s}^{-1}$ (Ref. 16). Since infinite viscosity also makes models using Equation 3-13 difficult to solve, COMSOL Multiphysics implements the power law model as

$$\mu = m \max(\dot{\gamma}, \dot{\gamma}_{\mathrm{min}})^{n-1} \tag{3-14}$$

where $\dot{\gamma}_{\mathrm{min}}$ is a lower limit for the evaluation of the shear rate magnitude. The default value for $\dot{\gamma}_{\mathrm{min}}$ is $10^{-2}\ \mathrm{s}^{-1}$, 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

$$\mu = \mu_{\infty} + (\mu_0 - \mu_{\mathrm{inf}})[1 + (\lambda\dot{\gamma})^2]^{\frac{(\mathrm{n}-1)}{2}} \tag{3-15}$$

where $\lambda$ is a parameter with the unit of time, $\mu_0$ is the zero shear rate viscosity, $\mu_{\mathrm{inf}}$ is the infinite shear-rate viscosity, and $\mathrm{n}$ is a dimensionless parameter. This expression is able to describe the viscosity for most stationary polymer flows.

### *The Boussinesq Approximation*

The Boussinesq approximation is a way to treat certain simple cases of buoyant flow without having to use the compressible formulation of the Navier-Stokes equations.

The Boussinesq approximation assumes that variations in density have no effect on the flow field except that they give rise to a buoyancy force. The density is assigned a reference value, $\rho_0$, everywhere except in the volume force term, which is set to

$$\mathbf{F} = (\rho_0 + \Delta\rho)\mathbf{g} \tag{3-16}$$

where $\mathbf{g}$ is the gravity vector. A further simplification is often possible. Because $\mathbf{g}$ can be written in terms of a potential, $\Phi$, Equation 3-16 can be written as:

$$\mathbf{F} = -\nabla(\rho_0\Phi) + \Delta\rho\mathbf{g}$$

The first part can be canceled out by splitting the true pressure, $p$, into a hydrodynamic component, $P$, and a hydrostatic component, $-\rho_0\Phi$. Equation 3-11 and Equation 3-12 are expressed in terms of the hydrodynamic pressure $P = p + \rho_0\Phi$:

$$\rho\nabla\cdot\mathbf{u} = 0 \tag{3-17}$$

$$\rho_0\frac{\partial\mathbf{u}}{\partial t}+(\rho_0\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla P+\nabla\cdot(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))+\mathbf{g}\Delta\rho \tag{3-18}$$

To obtain the Boussinesq approximation on this form, the flow must be defined as **Incompressible** with the **Include gravity** and **Use reduced pressure** options selected in the flow interface, and the **Nonisothermal Flow** multiphysics feature should be used to coupled the heat transfer and fluid flow interfaces.

In practice, the shift from $p$ to $P$ can be ignored except where the pressure appears in boundary conditions. The pressure that is specified at boundaries is the reduced pressure in this case. For example, at a vertical outflow or inflow boundary, the reduced pressure is typically a constant, whereas the true pressure is a function of the vertical coordinate.

The system formed by Equation 3-17 and Equation 3-18 has its limitations. The main assumption 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. An excellent discussion of the Boussinesq approximation and its limitations appears in Chapter 14 of Ref. 10.

## *Theory for the Wall Boundary Condition*

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:

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

The no-penetration term takes precedence over the Neumann part of the condition and the above expression is therefore equivalent to

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

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 $\mathbf{u}_{\mathrm{rel}} = \mathbf{u} - \mathbf{u}_{\mathrm{tr}}$.

The boundary condition for $\nu$ is $\nabla\tilde{\nu} \cdot \mathbf{n} = 0$.

### 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 $U_{\mathrm{w}}$ and the condition prescribes

  $$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{u} \cdot \mathbf{t} = U_{\mathrm{w}}$$

  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 $\mathbf{u}_{\mathrm{w}}$ projected onto the boundary plane:

  $$\mathbf{u} = \frac{\mathbf{u}_{\mathrm{w}} - (\mathbf{n} \cdot \mathbf{u}_{\mathrm{w}})\mathbf{n}}{\|\mathbf{u}_{\mathrm{w}} - (\mathbf{n} \cdot \mathbf{u}_{\mathrm{w}})\mathbf{n}\|}\|\mathbf{u}_{\mathrm{w}}\|$$

  The normalization makes $\mathbf{u}$ have the same magnitude as $\mathbf{u}_{\mathrm{w}}$ even if $\mathbf{u}_{\mathrm{w}}$ 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 $\beta$ is given by

$$\beta = \frac{\mu}{\left(\frac{2-\alpha_\mathrm{v}}{\alpha_\mathrm{v}}\right)\lambda}$$

where $\mu$ is the fluid's dynamic viscosity (SI unit: Pa·s), $\alpha_\mathrm{v}$ represents the tangential momentum accommodation coefficient (TMAC) (dimensionless), and $\lambda$ 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. 15.

A simpler expression for $\beta$ is

$$\beta = \frac{\mu}{L_s}$$

where $L_\mathrm{s}$, 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:

$$\Delta u = \sigma_\mathrm{T}\frac{\mu}{\rho}\nabla_t \log T$$

where $\sigma_\mathrm{T}$ is the thermal slip coefficient (dimensionless) and $\rho$ is the density of the fluid. The thermal slip coefficients range between 0.3 and 1.0 and can be found in Ref. 15.

Combining the previous relationships results in the following equation:

$$\mathbf{u} - \mathbf{u}_{\mathrm{w},t} = \frac{L_s}{\mu}\tau_{n,t} + \sigma_\mathrm{T}\frac{\mu}{\rho T}\nabla_t T$$

Relate the tangential shear stress to the viscous boundary force by

$$\tau_{n,t} = \mathbf{K} - (\mathbf{n}\cdot\mathbf{K})\mathbf{n}$$

where the components of **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.

## ELECTROOSMOTIC VELOCITY

Most solid surfaces acquire a surface charge when brought into contact with an electrolyte. In response to the spontaneously formed surface charge, a charged solution forms close to the liquid-solid interface. This is known as an electric double layer. If an electric field is applied to the fluid, this very narrow layer starts to move along the boundary.

It is possible to model the fluid’s velocity near the boundary using the Helmholtz-Smoluchowski relationship between the electroosmotic velocity $u$ and the applied electric field:

$$u = \mu_{eo}\mathbf{E}_t$$

where $\mu_{eo}$ is the electroosmotic mobility and $\mathbf{E}_t$ is the fluid electric field tangential to the wall.

### *Built-in Expression*

Use the Electroosmotic mobility $\mu_{eo}$ (SI unit: $m^2/(s{\cdot}V)$) Built-in expression to compute the electroosmotic mobility from:

$$\mu_{eo} = -\varepsilon_r\varepsilon_0\frac{\zeta}{\mu} \qquad (3\text{-}19)$$

Here $\varepsilon_r$ is the fluid’s relative permittivity, $\varepsilon_0$ the permittivity of free space (SI unit F/m), which is a predefined physical constant, $\zeta$ is the fluid’s zeta potential (SI unit: V), and $\mu$ the fluid’s dynamic viscosity (Pa·s). Typically $\mu_{eo} \approx 7\times10^{-8} m^2/(s{\cdot}V)$ and $\zeta \approx 100$ mV (see H. Bruus, *Theoretical Microfluidics*, Oxford University Press, 2008). See Wall for the node settings.

*Electro-osmotic Micromixer*: Application Library path **Microfluidics_Module/Micromixers/electroosmotic_mixer**

## *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:

$$-p + 2\mu\frac{\partial u_n}{\partial n} = F_n \tag{3-20}$$

where $\partial u_n/\partial n$ is the normal derivative of the normal velocity component. Equation 3-20 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 3-20 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 3-20, 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 permit 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 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

## *Laminar Inflow*

In order to prescribe a fully developed inlet velocity profile, this boundary condition adds a weak form contribution and constraints corresponding to unidirectional flow perpendicular to the boundary. The applied condition corresponds to the situation shown in Figure 3-1: a fictitious domain of length $L_{entr}$ is assumed to be attached to the inlet of the computational domain. The domain is an extrusion of the inlet boundary, which means that laminar inflow requires the inlet to be flat. The boundary condition uses the assumption that the flow in this fictitious domain is *fully developed laminar flow*. The “wall” boundary conditions for the fictitious domain is inherited from the real domain, Ω, unless the option to constrain outer edges or endpoints to zero is selected in which case the fictitious “walls” are no-slip walls.

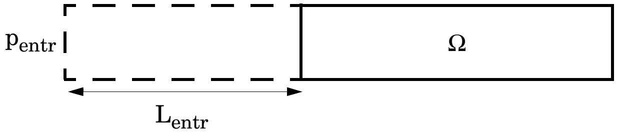

*Figure 3-1: An example of the physical situation simulated when using the Laminar inflow boundary condition. Ω is the actual computational domain while the dashed domain is a fictitious domain.*

If an average inlet velocity or inlet volume flow is specified instead of the pressure, COMSOL Multiphysics adds an ODE that calculates a pressure, $p_{entr}$, such that the desired inlet velocity or volume flow is obtained.

### *Laminar Outflow*

In order to prescribe an outlet velocity profile, this boundary condition adds a weak form contribution and constraints corresponding to unidirectional flow perpendicular to the boundary. The applied condition corresponds to the situation shown in Figure 3-2: assume that a fictitious domain of length $L_{exit}$ is attached to the outlet of the computational domain. The domain is an extrusion of the outlet boundary, which means that laminar outflow requires the outlet to be flat. The boundary condition uses the assumption that the flow in this fictitious domain is *fully developed laminar flow*. The “wall” boundary conditions for the fictitious domain is inherited from the real domain, Ω, unless the option to constrain outer edges or endpoints to zero is selected in which case the fictitious “walls” are no-slip walls.

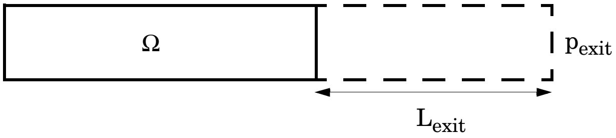

*Figure 3-2: An example of the physical situation simulated when using the Laminar outflow boundary condition. Ω is the actual computational domain while the dashed domain is a fictitious domain.*

If the average outlet velocity or outlet volume flow is specified instead of the pressure, the software adds an ODE that calculates $p_{exit}$ such that the desired outlet velocity or volume flow is obtained.

## *Mass Flow*

The **Mass Flow** boundary condition constrains the mass flowing into the domain across an inlet 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 $\rho$ is the density.

### MASS FLOW RATE

The mass flow rate boundary condition sets the total mass flow through the boundary according to:

$$-\int_{\partial\Omega} d_{bc}\rho(\mathbf{u}\cdot\mathbf{n})dS = m$$

where $d_{\mathrm{bc}}$ (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.

In addition to the constraint on the total flow across the boundary, the tangential velocity components are set to zero on the boundary

$$\mathbf{u}\times\mathbf{n} = \mathbf{0} \qquad (3\text{-}21)$$

### STANDARD FLOW RATE

The standard flow rate boundary condition specifies the mass flow as a standard volumetric flow rate. The mass flow through the boundary is set by the equation:

$$-\int_{\partial\Omega} d_{\mathrm{bc}}\frac{\rho}{\rho_{\mathrm{st}}}(\mathbf{u}\cdot\mathbf{n})dS = Q_{\mathrm{sv}}$$

where $d_{\mathrm{bc}}$ (only present in the 2D component Cartesian axis system) is the boundary thickness normal to the fluid-flow domain, $\rho_{\mathrm{st}}$ is the standard density, and $Q_{\mathrm{sv}}$ is the standard flow rate. The standard density is defined by one of the following equations:

$$\rho_{\mathrm{st}} = \frac{M_n}{V_n}$$

$$\rho_{\mathrm{st}} = \frac{p_{\mathrm{st}} M_n}{R T_{\mathrm{st}}}$$

where $M_n$ is the mean molar mass of the fluid, $V_n$ is the standard molar volume, $p_{\mathrm{st}}$ is the standard pressure, $R$ is the universal molar gas constant, and $T_{\mathrm{st}}$ is the standard temperature.

Equation 3-21 or Equation 3-22 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.

### *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

$$p = 2\mu\frac{\partial u_n}{\partial n} + f_0 \tag{3-22}$$

If $\partial u_n/\partial n$ is small, Equation 3-22 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

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -p_0\mathbf{n} \tag{3-23}$$

$$(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n} \tag{3-24}$$

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 3-23 or Equation 3-24 can be supplemented with a tangential velocity condition

$$\mathbf{u}\cdot\mathbf{t} = 0 \tag{3-25}$$

If so, the no-tangential-stress condition is overridden. An issue with Equation 3-23 or Equation 3-24 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

$$\begin{gathered}\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0\mathbf{n}\\ (-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0\mathbf{n}\\ \hat{p}_0\le p_0\end{gathered}\quad , \tag{3-26}$$

the normal stress is adjusted to keep

$$\mathbf{u}\cdot\mathbf{n}\ge 0 \tag{3-27}$$

Equation 3-26 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 3-26 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

$$\begin{gathered}\mathbf{n}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0\\ \mathbf{n}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0\\ \hat{p}_0\ge p_0\end{gathered} \tag{3-28}$$

together with the tangential condition in Equation 3-25, or, a general flow direction is prescribed.

$$\begin{gathered}\mathbf{r}_{\mathbf{u}}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n}=-\hat{p}_0(\mathbf{r}_{\mathbf{u}}\cdot\mathbf{n})\\ \mathbf{r}_{\mathbf{u}}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n}=-\hat{p}_0(\mathbf{r}_{\mathbf{u}}\cdot\mathbf{n})\\ \hat{p}_0\ge p_0\\ \mathbf{u}-(\mathbf{u}\cdot\mathbf{r}_{\mathbf{u}})\mathbf{r}_{\mathbf{u}}=\mathbf{0},\ \mathbf{r}_{\mathbf{u}}=\frac{\mathbf{d}_{\mathbf{u}}}{\|\mathbf{d}_{\mathbf{u}}\|}\end{gathered} \tag{3-29}$$

The “>” option is used with suppress backflow to have $\mathbf{u}\cdot\mathbf{n}\le 0$ or $\mathbf{u}\cdot\mathbf{r}_{\mathbf{u}}\ge 0$.

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.

## *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: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Microfluidics Module, Pipe 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 $\delta V$ 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

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q} = \dot{q}_\mathrm{p} \tag{3-30}$$

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 3-30, $\dot{Q}$ must tend to plus or minus infinity as $\delta V$ 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 3-30 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 $\delta S$ and then letting $\delta S$ 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

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_1 \qquad (3\text{-}31)$$

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

$$\dot{q}_1 \mathrm{test}(p)$$

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.

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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 Batteries & Fuel Cells 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 3-10 or Equation 3-12) 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** button ( ) and select **Stabilization**.

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. 7) and were later extended to Galerkin least-squares (GLS) applied to the Navier-Stokes equations (Ref. 8). This is the streamline diffusion formulation that COMSOL Multiphysics supports. The time-scale tensor is the diagonal tensor presented in Ref. 9.

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 Babuska-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. 8 with a shock-capturing viscosity of the Hughes-Mallet type Ref. 7.

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.

#### 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 Mutligrid (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, 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. 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 P2+P1 elements and P3+P2 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 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-$\alpha$ method instead. Generalized-$\alpha$ is a solver which has properties similar to those of the second-order BDF solver but it is much less diffusive.

Both BDF and generalized-$\alpha$ 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 3-12 reduces to:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F} \tag{3-32}$$

Solving Equation 3-32 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 3-32:

$$\rho\frac{\mathbf{u}-\mathrm{nojac}(\mathbf{u})}{\Delta\tilde{t}}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F}$$

where $\Delta\tilde{t}$ is a *pseudo time step*. Since **u**–`nojac`(**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 $\Delta\tilde{t}$ of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step $\Delta\tilde{t}$ can be chosen individually for each element based on the local CFL number:

$$\Delta\tilde{t} = \mathrm{CFL}_{\mathrm{loc}}\frac{h}{|\mathbf{u}|}$$

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 $\mathrm{CFL}_{\mathrm{loc}}$ 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 $\mathrm{CFL}_{\mathrm{loc}}$ as the solution comes closer to convergence.

The default manual expression is

$$\begin{gathered}1.3^{\min(\mathrm{niterCMP},\,9)}+\\ \mathrm{if}(\mathrm{niterCMP}>20,\,9\cdot 1.3^{\min(\mathrm{niterCMP}-20,\,9)},\,0)+\\ \mathrm{if}(\mathrm{niterCMP}>40,\,90\cdot 1.3^{\min(\mathrm{niterCMP}-40,\,9)},\,0)\end{gathered} \tag{3-33}$$

The variable `niterCMP` is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. $\mathrm{CFL}_{\mathrm{loc}}$ 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 3-33 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*.

## *Discontinuous Galerkin Formulation*

Some boundary conditions are implemented using a discontinuous Galerkin formulation. These boundary conditions include

- Wall – Slip, Sliding walls and moving walls (that is, walls with non-zero translational velocity).
- Periodic Flow Condition
- Flow Continuity

The formulation used in the Fluid Flow interfaces in COMSOL Multiphysics is 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. 13.

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 in COMSOL Multiphysics is implemented according to Ref. 14.

## *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. 11). 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, $\rho$ the fluid density, and $\mu$ 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.

## *References for the Single-Phase Flow, Laminar Flow Interfaces*

1. G.G. Stokes, Trans. Camb. Phil. Soc., 8, 287-305, 1845

2. P.M. Gresho and R.L. Sani, *Incompressible Flow and the Finite Element Method, Volume 2: Isothermal Laminar Flow*, John Wiley & Sons, 2000.

3. G.K. Batchelor, *An Introduction To Fluid Dynamics*, Cambridge University Press, 1967.

4. R.L. Panton, *Incompressible Flow*, 2nd ed., John Wiley & Sons, 1996.

5. I. Harari and T.J.R. Hughes, "What are $C$ and $h$? Inequalities for the Analysis and Design of Finite Element Methods," *Comp. Meth. Appl. Mech. Engrg*, vol. 97, pp. 157–192, 1992.

6. Y. Bazilevs, V.M. Calo, T.E. Tezduyar, and T.J.R. Hughes, "$YZ\beta$ Discontinuity Capturing for Advection-dominated Processes with Application to Arterial Drug Delivery," *Int.J.Num. Meth. Fluids*, vol. 54, pp. 593–608, 2007.

7. T.J.R. Hughes and M. Mallet, "A New Finite Element Formulation for Computational Fluid Dynamics: III. The Generalized Streamline Operator for Multidimensional Advective-Diffusive System," *Comp. Meth. Appl. Mech. Engrg*, vol. 58, pp. 305–328, 1986.

8. G. Hauke and T.J.R. Hughes, "A Unified Approach to Compressible and Incompressible Flows," *Comp. Meth. Appl. Mech. Engrg*, vol. 113, pp. 389–395, 1994.

9. G. Hauke, "Simple Stabilizing Matrices for the Computation of Compressible Flows in Primitive Variables," *Comp. Meth. Appl. Mech. Engrg*, vol. 190, pp. 6881–6893, 2001.

10. D.J. Tritton, *Physical Fluid Dynamics*, 2nd ed., Oxford University Press, 1988.

11. J.M. Coulson and J.F. Richardson, “Particle Technology and Separation Processes,” *Chemical Engineering, Volume 2*, Butterworth-Heinemann, 2002.

12. J.L. Guermond, P. Minev, and J. Shen, “An overview of projection methods for incompressible flows,” *Comp. Meth. Appl. Mech. Engrg*, vol. 195, pp. 6011–6045, 2006.

13. B. Rivière, *Discontinuous Galerkin Methods for Solving Elliptic and Parabolic Equations*, SIAM, 2008.

14. Y. Epshteyn and B. Rivière, “Estimation of penalty parameters for symmetric interior penalty Galerkin methods,” *J. Computational and Applied Mathematics*, vol. 206, pp. 843–872, 2007.

15. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

16. R.P. Chhabra and J.F. Richardson, *Non-Newtonian Flow and Applied Rheology*, 2nd ed., Elsevier, 2008.

# 4

# Multiphase Flow, Two-Phase Flow Interfaces

There are several Fluid Flow interfaces available with the Microfluidics Module. These are found under the **Fluid Flow>Multiphase Flow** branch ( ) when adding a physics interface. See Modeling Microfluidic Fluid Flows to help select the physics interface to use.

In this chapter:

# The Laminar Two-Phase Flow, Level Set and Laminar Two-Phase Flow, Phase Field Interfaces

This section includes the following topics:

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- Mathematics, Moving Interfaces

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## 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 the **Multiphysics** node, a multiphysics coupling feature **Two-Phase Flow, Level Set** is added automatically. Another multiphysics coupling feature **Wetted Wall** can be added when needed.

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

#### *Multiphysics Coupling Option*

Laminar Flow interface coupled to a Laminar Two-Phase Flow, Level Set interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar Two-Phase Flow, Level Set interface **Multiphysics coupling option** is automatically set to **Level Set**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \tag{4-1}$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces.

- Theory for the Level Set and Phase Field Interfaces
- Theory for the Single-Phase Flow Interfaces

## *The Turbulent Two-Phase Flow, Level Set Interface*

The **Turbulent 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 **Turbulent Two-Phase Flow, Level Set** multiphysics interface, a **Laminar Flow** and a **Level Set** interface are added to the Model Builder. In addition the **Multiphysics** node, a multiphysics coupling feature **Two-Phase Flow, Level Set** is added automatically. Another multiphysics coupling feature **Wetted Wall** can be added when needed.

Simulations using the Turbulent 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

*Multiphysics coupling option*

Laminar Flow interface coupled to a Laminar Two-Phase Flow, Level Set interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar Two-Phase Flow, Level Set interface **Multiphysics coupling option** is automatically set to **Level Set**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \tag{4-2}$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces.

- Theory for the Level Set and Phase Field Interfaces
- Theory for the Single-Phase Flow Interfaces

## *Two-Phase Flow, Level Set Coupling Features*

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 multiphysics coupling feature **Two-Phase Flow, Level Set** defines density and dynamic viscosity of the flow used in the **Laminar Flow** interfaces, and defines the surface tension on the interface in form of a volume force used in momentum equation. It also enable the **Level set** interface use the velocity field calculated from **Laminar Flow**interfaces to convect 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.

### FLUID PROPERTIES

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** $\rho_1$ and **Dynamic viscosity of fluid 1** $\mu_1$ are both set to **From Material**.

The non-Newtonian power-law and Carreau 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** $\rho_1$ or the **Dynamic viscosity of fluid 1** $\mu_1$ drop down list and enter the expression in the corresponding edit field.

Similarly, the properties of **Fluid 2** can be specified.

⚠ 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.

### SURFACE TENSION

Select the **Neglect surface tension in momentum equation** check box to neglect surface tension.

Select a **Surface tension coefficient** $\sigma$ (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**, **Glycerol/Air** and so forth).
- For **User defined** enter a value or expression for the surface tension coefficient $\sigma$ (SI unit: N/m).

#### 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.

## *The Wetted Wall Coupling Feature*

The **Laminar Two-Phase Flow, Level Set,** () interfaces contain an optional multiphysics coupling boundary feature, **Wetted Wall**. It is an exclusive feature which overrides the **Wall** feature of Laminar Flow or Turbulence Flow interfaces together with the **No Flow** feature of Level Set interface.

The **Wetted wall** boundary condition is suitable for walls in contact with the fluid-fluid interface. If this boundary condition is used, the fluid-fluid interface can move along the wall.

This boundary condition enforces the no-penetration condition $\mathbf{u}\cdot\mathbf{n}_{\mathrm{wall}} = 0$ and adds a frictional force of the form

$$\mathbf{F}_{\mathrm{fr}} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\beta$ is the slip length. For numerical calculations it is suitable to set $\beta = h$, 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 $\beta$ outside the wall (see Figure 4-1).

Finally, the boundary condition adds the following weak boundary term:

$$\int_{\partial\Omega} \mathrm{test}(\mathbf{u})\cdot[\sigma(\mathbf{n}_{\mathrm{wall}} - (\mathbf{n}\cos\theta_{\mathrm{w}}))\delta]\,dS$$

The boundary term results from the partial integration of the surface tension force in the momentum equation. Define the contact angle $\theta_w$ (that is, the angle between the fluid interface and the wall). Figure 4-1 illustrates the definition of the contact angle.

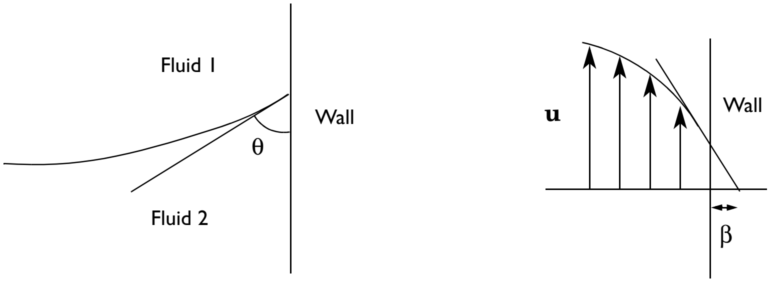

*Figure 4-1: Definition of the contact angle* $\theta$ *at interface/wall contact points (left) and an illustration of the slip length* $\beta$ *(right).*

### SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first multiphysics coupling feature **Wetted Wall** in the model) is ww1.

### 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.

#### 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.

#### WETTED WALL

Here define the following two properties for the wetted wall:

- Enter a value or expression for the **Contact angle** $\theta_w$. The default is `pi/2` ($\pi/2$) rad.
- Enter a value or expression for the **Slip length** $\beta$ (SI unit: m). The default is `h`, which is the variable for the local mesh element size $h$.

- Theory for the Level Set and Phase Field Interfaces

## *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** interface are added to the Model Builder. In addition the **Multiphysics** node, a multiphysics coupling feature **Two-Phase Flow, Phase Field** is added automatically. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall function here is not implemented as a separated multiphase coupling boundary feature, but as the default **Wetted Wall** feature of **Phase Field** interface.

Wetted Wall

Simulations using the Laminar Two-Phase Flow, Phase Field interface are always time-dependent since the position of an interface is almost always dependent on its history.

### INTERFACE PROPERTIES

#### *Multiphysics Coupling Option*

Laminar Flow interface coupled to a Laminar Two-Phase Flow, Phase Field interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar Two-Phase Flow, Phase Field interface, a **Multiphysics coupling option** is automatically set to **Phase Field**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \qquad (4\text{-}3)$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces

Theory for the Two-Phase Flow Interfaces

## *The Turbulent Two-Phase Flow, Phase Field Interface*

The **Turbulent 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 **Turbulent Two-Phase Flow, Phase Field** multiphysics interface, a **Turbulent Flow** and a **Phase Field** interface are added to the Model Builder. In addition the **Multiphysics** node, a multiphysics coupling feature **Two-Phase Flow, Phase Field** is added automatically. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall function here is not implemented as a separated multiphase coupling boundary feature, but as the default **Wetted Wall** feature of **Phase Field** interface.

Wetted Wall

Simulations using the Laminar Two-Phase Flow, Phase Field interface are always time-dependent since the position of an interface is almost always dependent on its history.

### INTERFACE PROPERTIES

#### *Multiphysics Coupling Option*

Laminar Flow interface coupled to a Laminar Two-Phase Flow, Phase Field interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Laminar Two-Phase Flow, Phase Field interface, a **Multiphysics coupling option** is automatically set to **Phase Field**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\nabla \cdot \mathbf{u} = 0 \tag{4-4}$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces

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Theory for the Two-Phase Flow Interfaces

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## *The Two-Phase Flow, Phase Field Coupling Features*

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 multiphysics coupling feature **Two-Phase Flow, Phase Field** defines density and dynamic viscosity of the flow used in the **Laminar Flow** and **Turbulent Flow** interfaces, and defines the surface tension on the interface in form of a volume force used in momentum equation. It also enable the **Phase Field** interface use the velocity field calculated from **Laminar Flow** or **Turbulent Flow** interfaces to convect 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.

### FLUID PROPERTIES

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** $\rho_1$ and **Dynamic viscosity of fluid 1** $\mu_1$ are both set to **From Material**.

The non-Newtonian power-law and Carreau 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** $\rho_1$ or the **Dynamic viscosity of fluid 1** $\mu_1$ drop down list and enter the expression in the corresponding edit field.

Similarly, the properties of **Fluid 2** can be specified.

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⚠ Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2.

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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.

### SURFACE TENSION

Select the **Neglect surface tension in momentum equation** check box to neglect surface tension.

Select a **Surface tension coefficient** $\sigma$ (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**, **Glycerol/Air** and so forth).
- For **User defined** enter a value or expression for the surface tension coefficient $\sigma$ (SI unit: N/m).

### 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 Level Set and Phase Field Interfaces

## *Domain, Boundary, Point, and Pair Nodes for the Laminar 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 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.

### LEVEL SET

The available physics features for the Level Set Interface are listed in Domain, Boundary, and Pair Nodes for the Level Set Interface.

### PHASE FIELD

The available physics features for the Phase Field Interface are listed in Domain, Boundary, and Pair Nodes for the 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 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

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- Mathematics, Moving Interfaces

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## *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, to be of 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.

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The Multiphysics Node in the *COMSOL Multiphysics Reference Manual*.

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Simulations using the Laminar Three-Phase Flow, Phase Field interface are always time-dependent since the position of an interface is almost always dependent of its history.

### INTERFACE PROPERTIES

#### *Turbulence Model*

Since the Three-Phase Flow, Phase Field interface assumes laminar flow, the Turbulence Model property in the Laminar Flow interface is deactivated when the interface is added as a part of a multiphysics interface.

#### *Multiphysics Coupling Option*

Laminar Flow interfaces coupled to a Three-Phase Flow, Phase Field interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Three-Phase Flow, Phase Field interface **Multiphysics coupling option** is automatically set to **Ternary Phase Field**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\frac{\partial \log\rho}{\partial t} + \nabla\cdot\mathbf{u} + \mathbf{u}\cdot\nabla\log\rho = 0 \qquad (4\text{-}5)$$

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces.

## *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.

### FLUID PROPERTIES

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** $\rho_A$ and **Dynamic viscosity of fluid A** $\mu_A$ are both set to **From Material**.

The non-Newtonian power-law and Carreau 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** $\rho_A$ or the **Dynamic viscosity of fluid A** $\mu_A$ drop down list and enter the expression in the corresponding edit 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.

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- Theory for the Level Set and Phase Field Interfaces

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## *Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface*

The Laminar Three-Phase Flow, Phase Field Interface is a multiphysics interface combining The Laminar Flow Interface and the The Ternary Phase Field Interface.

### 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 Ternary Phase Field Interface 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 (tpfmm)** interface (), found under the **Multiphase Flow>Two-Phase Flow, Moving Mesh** branch () when adding a physics interface, has the domain level equations and boundary conditions 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.

The main node is the Fluid Properties feature, which adds the Navier-Stokes equations and provides an interface for defining the properties of the fluids and the surface tension. 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).

The following default nodes are added when using this physics interface—**Free Deformation**, **Prescribed Mesh Displacement**, **Wall**, **Initial Values**, and **Fluid Properties**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Laminar Two-Phase Flow, Moving Mesh** 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 `tpfmm`.

### PHYSICAL MODEL

This physics interface deforms the mesh within the domains on either side of the two fluid interface to track its movement.

The **Compressibility** defaults to **Compressible flow (Ma<0.3)**, which uses a compressible formulation of the Navier-Stokes equations. Select **Incompressible flow** to use the incompressible (constant density) 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)** check box, which significantly improves the solver speed.

Enter a **Reference pressure level** $p_{\mathrm{ref}}$ (SI unit: Pa). The default value is `1[atm]`.

### FREE DEFORMATION SETTINGS

Select a **Mesh smoothing type** — **Winslow** (the default), **Laplace**, **Hyperelastic**, or **Yeoh**. For the Yeoh mesh smoothing type, also specify a **Stiffening factor** (default: 100). See Smoothing Methods in the *COMSOL Multiphysics Reference Manual* for more information.

### FRAME SETTINGS

The **Material frame coordinates** setting enables the names of the space coordinates for tracking the mesh movement in the **x**, **y**, and **z** directions to be changed. The default names are the coordinates of the spatial frame in uppercase letters.

The **Geometry shape order** setting controls the order of polynomials used for representing the geometry shape in the spatial frame. The same order is used for Lagrange shape functions defining the mesh position in domains where the Free displacement option has been activated.

### 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.

| | |
|---|---|
| ! | In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 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, Edge, Point, and Pair Nodes for the Laminar Two-Phase Flow, Moving Mesh Interface
- Smoothing Methods in the *COMSOL Multiphysics Reference Manual*

The following models are found at this Application Library path **Microfluidics_Module/Two_Phase_Flow>[file name]**

- *Jet Instability—Moving Mesh*: **jet_instability**
- *Electrowetting Lens*: **electrowetting_lens**
- *The Viscous Catenary*: **viscous_catenary**

## *Domain, Boundary, Edge, Point, and Pair Nodes for the Laminar Two-Phase Flow, Moving Mesh Interface*

The Laminar Two-Phase Flow, Moving Mesh Interface 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.

Boundary conditions (and edge and point nodes) must be specified for the moving mesh on all external boundaries of the model. It can also be beneficial to set boundary conditions on internal boundaries - depending on the problem and the geometry. The boundary conditions are of two forms: a **Prescribed Mesh Displacement** and a **Prescribed Mesh Velocity**.

These nodes are described in this section (listed in alphabetical order):

- External Fluid Interface
- Fluid-Fluid Interface
- Fixed Mesh
- Free Deformation
- Initial Values
- Navier Slip
- Prescribed Mesh Displacement
- Prescribed Mesh Velocity
- Wall
- Wall-Fluid Interface

These nodes are described for the Moving Mesh interface in the *COMSOL Multiphysics Reference Manual* (listed in alphabetical order):

- Prescribed Deformation
- Prescribed Normal Mesh Velocity
- Zero Normal Mesh Displacement
- Zero Normal Mesh Velocity

These nodes are described for the Laminar Flow interface (listed in alphabetical order):

- Flow Continuity
- Fluid Properties
- Inlet
- No Viscous Stress
- Open Boundary
- Outlet
- Periodic Flow Condition
- Pressure Point Constraint
- Symmetry
- Volume Force

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Smoothing Methods in the *COMSOL Multiphysics Reference Manual*

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In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 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.

## *Free Deformation*

The **Free Deformation** default node applies the equations for the moving mesh to the domains selected, to allow deformation of the mesh. Domains either side of a fluid-fluid interface must have this option selected.

### INITIAL DEFORMATION

Enter values or expressions for each coordinate based on the space dimension for the **Initial mesh displacement** ($dx_0$, $dy_0$, $dz_0$) (SI unit: m). The default is for no mesh displacement.

## *Prescribed Mesh Displacement*

The **Prescribed Mesh Displacement** boundary condition fixes the mesh displacement to a constant value (typically 0). The displacement can be fixed along the global coordinate axis or by using another boundary system. In particular the boundary coordinate system is useful and can be employed to specify a zero displacement perpendicular to the boundary (if, for example, the boundary represents a solid wall). Often it is desirable to constrain the mesh displacement only in one direction (for example perpendicular to but not parallel to a solid boundary). In this case, click to clear the check box next to the prescribed displacement if the free axis should be deselected.

If a Fluid-Fluid Interface is in contact with a solid boundary the mesh displacement parallel to the boundary cannot be fixed if the contact point is moving. In this case the Navier Slip boundary condition and the Prescribed Mesh Displacement boundary condition (with displacement prescribed only in the normal direction) represent a suitable choice of boundary conditions.

### PRESCRIBED MESH DISPLACEMENT

By default the **Prescribed x mesh displacement**, **Prescribed y mesh displacement**, and **Prescribed z mesh displacement** check boxes are selected. The available fields are based on the space dimension of the model. Enter values or expressions for each of the **Prescribed mesh displacement** fields $dx$, $dy$, and $dz$ (SI unit: m). Click to clear the check boxes as needed.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

## Initial Values

The **Initial Values** nod 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 values or expressions for the initial value of the **Velocity field** u (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0.

## Fixed Mesh

The **Fixed Mesh** node specifies that the mesh does not move in the selected domains. A fixed mesh should only be used on domains that are not adjacent to a fluid-fluid interface.

> ⚠ All the elements on the domain boundary are also fixed. Care should be taken to prevent mesh movement in an undesirable manner in an adjacent free deformation domain.

## Prescribed Mesh Velocity

The **Prescribed Mesh Velocity** boundary condition is used to set the mesh velocity rather than the mesh displacement. This boundary condition is applied automatically to fluid-fluid interfaces (where the mesh velocity is set to the fluid velocity). It might also be used to model, for example, a moving wall.

Note these limitations for the Moving Mesh:

- The connectivity of the mesh remains unchanged during the mesh deformation, which means that topological changes in the geometry (for example, a droplet pinch off) cannot be simulated.
- When the mesh deformation becomes large, the quality of the mesh created by the smoothing equations can deteriorate. If this happens, the solver runs into convergence problems. Sometimes the warning **Inverted mesh element** is displayed in the Progress window for the solver, which means that a mesh element has

(partially) warped inside-out. In this case introducing extra boundaries with explicit deformation inside the domains can help. Using a quadrilateral mesh (which is typically stiffer as it deforms) is another possibility. Also generate a new mesh for the region covered by the deformed mesh and let the solver continue by deforming the new mesh; see Remeshing a Deformed Mesh in the *COMSOL Multiphysics Reference Manual*.

- When using **Geometry shape order** larger than 1 in the Moving Mesh and Deformed Geometry interfaces, the mesh moving techniques often produce elements with distorted shapes. The default value of 1 is appropriate for most situations, provided a sufficiently fine mesh is employed.

The measure of mesh quality does not capture these distorted shapes because it is computed from the positions of the corners of the mesh element (ignoring midsize nodes, for example).

### PRESCRIBED MESH VELOCITY

By default the **Prescribed x velocity**, **Prescribed y velocity**, and **Prescribed z velocity** check boxes are selected. The available fields are based on the space dimension of the model. Enter values or expressions for each of the **Prescribed mesh velocity** fields $v_x$, $v_y$, and $v_z$ (SI unit: m/s). Click to clear the check boxes as needed.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

- Prescribed Mesh Displacement
- Weak Constraint and Deformed Geometry and Moving Mesh 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 Wall-Fluid Interface subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### SURFACE TENSION

The default **Surface tension coefficient** $\sigma$ (SI unit: N/m) is **User defined**. Or select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**.

- For **Library coefficient, liquid/gas interface** select an option from the list—**Water/Air**, **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**.

### 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: $\mathrm{kg/(m^2 \cdot s)}$) 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.

## *External Fluid Interface*

The **External Fluid Interface** 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. It also includes equations to model the interface. The Wall-Fluid Interface subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### FREE SURFACE

Enter an **External pressure** $p_{\mathrm{ext}}$ (SI unit: Pa).

#### SURFACE TENSION

The default **Surface tension coefficient** $\sigma$ (SI unit: N/m) is **User defined**. Or select **Library coefficient, liquid/gas interface** or **Library coefficient, liquid/liquid interface**.

- For **Library coefficient, liquid/gas interface** select an option from the list: **Water/Air**, **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**.

## *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/or asymptotic expressions for certain turbulence variables.

#### BOUNDARY CONDITION

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

- No Slip
- Slip
- Sliding Wall
- Moving Wall
- Leaking Wall
- Electroosmotic Velocity
- Slip Velocity

### *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.

### *Sliding Wall*

The **Sliding wall** boundary condition 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** $\mathbf{u}_\mathrm{w}$ 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** $U_\mathrm{w}$ should be specified in 2D.
- For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the **Velocity of moving wall**, $\varphi$ **component** $v_\mathrm{w}$ may also be specified.

### *Moving Wall*

For an arbitrary wall movement, the condition $\mathbf{u} = \mathbf{u}_\mathrm{w}$ may be prescribed. In this case, the components of the **Velocity of moving wall** $\mathbf{u}_\mathrm{w}$ should be specified.

Specifying this boundary condition 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.

### *Leaking Wall*

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

### *Electroosmotic Velocity*

When an electric field drives a flow along the boundary, the components for the **Electric field** $\mathbf{E}$ along with the **Electroosmotic mobility** $\mu_\mathrm{eo}$ should be defined. The **Built-in expression** for the **Electroosmotic mobility** requires values or expressions for the **Zeta potential** $\zeta$ and the **Relative permittivity** $\varepsilon_\mathrm{r}$

This option requires the Microfluidics Module.

### *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. The components of **Velocity of moving wall:** $\mathbf{u}_\mathrm{w}$ should be specified. Zero values are used for a stationary wall.

When the **Use viscous slip** check box is selected, the default **Slip length** $L_\mathrm{s}$ 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** $\alpha_\mathrm{v}$ and the **Mean free path** $\lambda$ 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** check box is selected, a thermal creep contribution with **Thermal slip coefficient** $\sigma_T$ 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.

This boundary condition is not compatible with the projection method.

### CONSTRAINT SETTINGS

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

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

## *Wall-Fluid Interface*

The **Wall Fluid Interface** subnode is available from the context menu (right-click the Fluid-Fluid Interface and External Fluid Interface parent node) or from the **Physics** toolbar, **Attributes** menu. This feature applies the forces necessary to maintain the contact angle at the wall.

| | |
|---|---|
| ! | The **Wall-Fluid Interface** node should only be used with the Navier Slip boundary condition, which should be applied to the adjacent wall(s). If another boundary condition is used with this feature the normal for the wall is not correct on the wall-fluid interface, leading to an incorrect force on the contact line. |

### WALL-FLUID INTERFACE

Select an option from the **Specify contact angle list** — **Directly** (the default) or **Through Young's equation**.

- For **Directly** enter a **Contact angle** $\theta_w$ (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** $\gamma_{s1}$ (SI unit: J/m$^2$) and **Phase 2-Solid surface energy density** $\gamma_{s2}$ (SI unit: J/m$^2$).

| | |
|---|---|
| | The contact angle $\theta_w$ is defined between the fluid-fluid interface and the surface of the wall adjacent to phase 1. |

## *Navier Slip*

The **Navier Slip** boundary condition is suitable for walls in contact with the fluid-fluid interface. If this boundary condition is used in combination with a **Prescribed Displacement** perpendicular to the wall only, the fluid-fluid interface can move along the wall. For applications where the interface is fixed on the wall, the **Wall-No slip** condition together with a zero **Prescribed Displacement** both parallel and perpendicular to the wall can be used.

The boundary condition enforces the slip condition $\mathbf{u}\cdot\mathbf{n}_{\text{wall}} = 0$ and adds a frictional force of the form

$$\mathbf{F}_{\text{fr}} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\beta$ is the slip length. By default $\beta = h/5$, where $h$ is the mesh element size. Strictly speaking the slip length should be set to a fixed physically motivated value (which is typically a few 10 s of nm) and the mesh should be fine enough to resolve distances of the order of the slip length. For many practical purposes the above approximation is sufficient. This boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at the distance β outside the wall (this is illustrated for the wetted wall boundary condition in Figure 4-2).

For axisymmetric components when the Swirl flow property is active, there is an option to set a value for the **Out-of-plane wall velocity**, $v_w$. In this case, an additional constraint is imposed on the φ component of the velocity:

$$u_{\varphi} = v_w$$

### NAVIER SLIP

Enter a **Slip length** $\beta$ (SI unit: m).

Select **Stationary wall** (the default) or **Normal wall velocity** to specify whether the wall is stationary or moving. In the case of Normal wall velocity the **Wall velocity** (m/s) should be entered. For axisymmetric components when the **Swirl flow** property is active there is the option to select **Out-of-plane wall velocity** and enter the **Velocity of moving wall, φ component.** The **Swirl flow** property in the Two-phase Flow, Moving Mesh interface requires both the CFD and Microfluidics Modules.

! The moving mesh boundary condition must be compatible with the motion of the wall for the problem to have a valid solution.

# Theory for the Level Set and Phase Field 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 Laminar Two-Phase Flow, Level Set and Laminar Two-Phase Flow, 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:

$$\rho\frac{\partial\mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+\nabla\mathbf{u}^T)]+\mathbf{F}_{\mathrm{g}}+\mathbf{F}_{\mathrm{st}}+\mathbf{F}_{\mathrm{ext}}+\mathbf{F} \tag{4-6}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{4-7}$$

Note that Equation 4-6, and Equation 4-7 are solved in the contained interface, **Laminar Flow** or **Turbulent Flow** interface. Note that if the Laminar Flow and Turbulent Flow are added automatically when we add a Two-Phase Flow, Level Set and Phase Field multiphysics interface, these interfaces contain a **Multiphysics coupling option** property to control the form of the continuity equation. The **Multiphysics coupling option** is automatically set to **Level Set** or **Phase Field**. In this case, the continuity equation takes the form as in Equation 4-7. When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the single-phase flow.

### USING THE LEVEL SET METHOD

If the level set method is used to track the interface, it adds the following equation:

$$\frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = \gamma\nabla \cdot \left(\varepsilon\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right) \tag{4-8}$$

where $\gamma$ is the reinitialization parameter (set to 1 by default), and $\varepsilon$ is the interface thickness controlling parameter (set to $h_{\mathrm{max}}/2$ where $h_{\mathrm{max}}$ is the maximum element size in the component). The density is a function of the level set function defined as

$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$

and the dynamic viscosity is given by

$$\mu = \mu_1 + (\mu_2 - \mu_1)\phi$$

where $\rho_1$ and $\rho_2$ are the constant densities of Fluid 1 and Fluid 2, respectively, and $\mu_1$ and $\mu_2$ are the dynamic viscosities 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 $\phi > 0.5$.

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:

$$\frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = \nabla \cdot \frac{\gamma\lambda}{\varepsilon^2}\nabla\psi \tag{4-9}$$

$$\psi = -\nabla \cdot \varepsilon^2\nabla\phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f_{\mathrm{ext}}}{\partial\phi} \tag{4-10}$$

where the quantity $\lambda$ (SI unit: N) is the mixing energy density and $\varepsilon$ (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, $\sigma$ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon}$$

and $\gamma$ is related to $\varepsilon$ through $\gamma=\chi\varepsilon^2$ where $\chi$ is the mobility tuning parameter (set to 1 by default). The volume fraction of Fluid 2 is computed as

$$V_{\mathrm{f}} = \min(\max([(1+\phi)/2], 0), 1)$$

where the `min` and `max` operators are used so that the volume fraction has a lower limit of 0 and an upper limit of 1. The density is then defined as

$$\rho = \rho_1 + (\rho_2 - \rho_1)V_f$$

and the dynamic viscosity according to

$$\mu = \mu_1 + (\mu_2 - \mu_1)V_f$$

where $\rho_1$ and $\rho_2$ are the densities and $\mu_1$ and $\mu_2$ 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:

$$G = \lambda\left(-\nabla^2\phi + \frac{\phi(\phi^2-1)}{\varepsilon^2}\right) + \frac{\partial f}{\partial\phi}$$

Details of the theory for the phase field method are in Ref. 2.

### FORCE TERMS

The four forces on the right-hand side of Equation 4-6 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 $\mathbf{F}_{st} = \sigma\kappa\delta\mathbf{n}$ where $\sigma$ is the surface tensions coefficient (SI unit: N/m), $\kappa$ is the curvature, and $\mathbf{n}$ is the unit normal to the interface. $\delta$ (SI unit: 1/m) is a Dirac delta function located at the interface. $\kappa$ depends on second derivatives of the level set function $\phi$. This can lead to poor accuracy of the surface tension force. Therefore, the following alternative formulation is used:

$$\mathbf{F}_{st} = \nabla\cdot(\sigma(\mathbf{I} - (\mathbf{n}\mathbf{n}^T))\delta)$$

For a derivation of this formulation, see Appendix A in Ref. 3. In the weak formulation of the momentum equation, it is possible to move the divergence operator, using integration by parts, to the test functions for the velocity components.

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

$$F_{\mathrm{st}} = \left(G - \frac{\partial f}{\partial\phi}\right)\nabla\phi$$

where $G$ is the chemical potential (SI unit: $\mathrm{J/m^3}$) defined in The Equations for the Phase Field Method and $\partial f/\partial\phi$ is a user-defined source of free energy.

### The Gravity Force

The gravity force is $\mathbf{F}_{\mathrm{g}} = \rho\mathbf{g}$ 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:

$$\mathbf{F}_{\mathrm{ext}} = \left(\frac{\partial f}{\partial\phi}\right)\nabla\phi$$

This force is added when a $\phi$ -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.

## 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 >, $D_{\mathrm{wi}}$. 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 4-8, Equation 4-9, and Equation 4-10 for a straight, non-moving interface.

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! For the initialization to work it is crucial that there are two **Initial Values** nodes and one **Initial Interface** node. One of the Initial Values nodes should use **Domain Initially: Fluid 1(ϕ =0)**and the other **Fluid initially in domain: Fluid 2(ϕ =0)**. The **Initial Interface** node is not default but can be added which should have all interior boundaries where the interface is initially present as selection. If the selection of the **Initial Interface** node is empty, the initialization fails. Note that the default value of **Domain Initially** is **Specified level set function explicitly** allowing arbitrary user defined initial value. In this case, no **Initial Interface** node should be added, and Time-dependent study should be used instead of Transient with Phase Initialization.

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- The Laminar Two-Phase Flow, Level Set and Laminar Two-Phase Flow, Phase Field Interfaces
- Studies and Solvers and Transient with Phase Initialization in the *COMSOL Multiphysics Reference Manual*

### Numerical Stabilization

Four types of stabilization methods are available for the flow (Navier-Stokes) and interface (level set or phase field) equations. Two are consistent stabilization methods — Streamline diffusion and Crosswind diffusion — and two are inconsistent — Isotropic diffusion and Anisotropic diffusion.

To display this section, click the **Show** button ( ) and select **Stabilization**.

- Theory for the Level Set and Phase Field Interfaces
- Stabilization in the *COMSOL Multiphysics Reference Manual*

### References for the Level Set and Phase Field Interfaces

1. E. Olsson and G. Kreiss, “A Conservative Level Set Method for Two Phase Flow”, *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

2. P. Yue, J.J. Feng, C. Liu, and J. Shen, “A Diffuse-interface Method for Simulating Two-phase Flows of Complex Fluids”, *J. Fluid Mech.*, vol. 515, pp. 293–317, 2004.

3. B. Lafaurie, C. Nardone, R. Scardovelli, S. Zaleski, and G. Zanetti “Modelling Merging and Fragmentation in Multiphase Flows with SURFER.”, *J. Comput. Phys.*, vol. 113, no. 1, pp. 134–147, 1994.

# Theory for the Three-Phase Flow, Phase Field 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 Laminar Three-Phase Flow, Phase Field Interface 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

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] + \mathbf{F}_{\mathrm{st}} + \mathbf{F} \qquad (4\text{-}11)$$

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

$$\frac{\partial \log\rho}{\partial t} + \nabla\cdot\mathbf{u} + \mathbf{u}\cdot\nabla\log\rho = 0 \qquad (4\text{-}12)$$

## 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

$$\begin{aligned}\frac{\partial\phi_i}{\partial t}+\nabla\cdot(\mathbf{u}\phi_i)&=\nabla\cdot\left(\frac{M_0}{\Sigma_i}\nabla\eta_i\right)\\ \eta_i&=\frac{4\Sigma_{\mathrm{T}}}{\varepsilon}\sum_{j\neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial\phi_i}-\frac{\partial F}{\partial\phi_j}\right)\right)-\frac{3}{4}\varepsilon\Sigma_j\nabla^2\phi_i\end{aligned}\tag{4-13}$$

governing the phase field variable, $\phi_i$, and a generalized chemical potential, $\eta_i$, 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

$$\sum_{i=A,B,C}\phi_i = 1\tag{4-14}$$

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 4-14, two sets of the equations shown in Equation 4-13 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 4-14.

The density and viscosity of the fluid mixture used in Equation 4-6 and 4-7 are defined as:

$$\begin{aligned}\rho&=\rho_A\phi_A+\rho_B\phi_B+\rho_C\phi_C\\ \mu&=\mu_A\phi_A+\mu_B\phi_B+\mu_C\phi_C\end{aligned}\tag{4-15}$$

### *Free energy*

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$F = \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 + \\ \phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2 \tag{4-16}$$

Here the $\sigma_{ij}$ denotes the surface tension coefficient of the interface separating phase $i$ and $j$, and the capillary parameters $\Sigma_i$ are defined for each phase in the manner of:

$$\begin{aligned} \Sigma_A &= \sigma_{AB} + \sigma_{AC} - \sigma_{BC} \\ \Sigma_B &= \sigma_{AB} + \sigma_{BC} - \sigma_{AC} \\ \Sigma_C &= \sigma_{BC} + \sigma_{AC} - \sigma_{AB} \end{aligned} \tag{4-17}$$

$\Lambda$ in the free energy is a function or parameter specifying the additional free bulk energy of the system. By default $\Lambda$ is zero. In this case it can be seen that the free energy in Equation 4-16 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 4-13, $\varepsilon$ (SI unit: 1/m) is a parameter controlling the interface thickness, $M_0$ (SI unit: $\mathrm{m}^3/\mathrm{s}$) is a molecular mobility parameter, and the parameter $\Sigma_T$ is defined as

$$\frac{3}{\Sigma_T} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \tag{4-18}$$

When using the interface it is recommended that the parameter $\varepsilon$ 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 a apply a mobility parameter such that the following holds approximately

$$M_0 = L_c U_c \varepsilon \cdot 10^{-2} \tag{4-19}$$

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 4-6) as a body force computed from the generalized chemical potentials:

$$\mathbf{F}_{\mathrm{st}} = \sum_{i = \mathrm{A}, B, C} \eta_i \nabla \phi_i \tag{4-20}$$

## *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
- Wall Fluid Interface 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:

- $\rho$ is the density (SI unit: $\text{kg/m}^3$)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- $p$ is pressure (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: $\text{N/m}^3$)

- $\tau$ is the viscous stress tensor (SI unit: Pa).

For a Newtonian fluid the viscous stress tensor, $\tau$, is given by:

$$\tau = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \tag{4-21}$$

The dynamic viscosity $\mu$ (SI unit: Pa·s) is allowed to depend on the thermodynamic state but not on the velocity field.

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Theory for the Single-Phase Flow Interfaces

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## *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.

For the Two-Phase Flow, Moving Mesh 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.

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Deformed Geometry and Moving Mesh in the *COMSOL Multiphysics Reference Manual*

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## *About the Fluid Interface Boundary Conditions*

The interfaces between phases are tracked with specific boundary conditions for the mesh displacement and the fluid flow. Two options are available—External Fluid Interface and Fluid-Fluid Interface. The External Fluid Interface 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 4-2), are given by (Ref. 1):

$$\mathbf{u}_1 = \mathbf{u}_2 + \left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right) M_f \mathbf{n}_i \tag{4-22}$$

$$\mathbf{n}_i \cdot \tau_2 = \mathbf{n}_i \cdot \tau_1 + \mathbf{f}_{st} \tag{4-23}$$

$$\mathbf{u}_{mesh} = \left(\mathbf{u}_1 \cdot \mathbf{n}_i - \frac{M_f}{\rho_1}\right)\mathbf{n}_i \tag{4-24}$$

where $\mathbf{u}_1$ and $\mathbf{u}_2$ are the velocities of the fluids 1 and 2 respectively, $\mathbf{u}_{mesh}$ 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), $\tau_1$ and $\tau_2$ 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)).

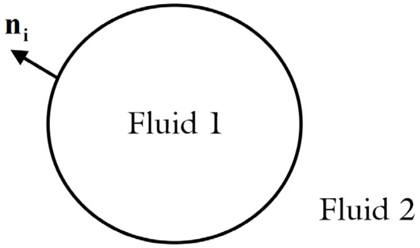

*Figure 4-2: Definition of fluid 1 and fluid 2 and the interface normal.*

The tangential components of Equation 4-22 enforce a no-slip condition between the fluids at the boundary. In the absence of mass transfer across the boundary, Equation 4-22 and Equation 4-24 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, $\tau_{uv}$, represent the $u^{\text{th}}$ 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 4-23 therefore expresses the force balance on the interface between the two fluids.

Two boundary conditions (Equation 4-22 and Equation 4-23) 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:

$$\mathbf{f}_{st} = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i - \nabla_s\sigma \tag{4-25}$$

where $\nabla_s$ 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 $\sigma$ is the surface tension at the interface.

In the two dimensional case it is straightforward to see the physical origin of Equation 4-25. Consider an element of the surface of unit depth into the page as shown in Figure 4-3. 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 4-25 is related to the mean curvature, $\kappa$, 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 4-25 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 4-3 can be obtained from the force balance along the direction of $\delta s$ 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 4-25.

To obtain additional insight into the boundary condition, it is helpful to re-write Equation 4-23 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 $\mu_1$ and $\mu_2$ 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

$$p_1 - p_2 + \mathbf{n}_i \cdot (\mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T) - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T)) \cdot \mathbf{n}_i = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i \qquad (4\text{-}26)$$

whereas in the tangential direction, $\mathbf{t}_i$,

$$\mathbf{n}_i \cdot (\mu_2(\nabla\mathbf{u}_2 - (\nabla\mathbf{u}_2)^T) - \mu_1(\nabla\mathbf{u}_1 - (\nabla\mathbf{u}_1)^T)) \cdot \mathbf{t}_i = |\nabla_s\sigma| \qquad (4\text{-}27)$$

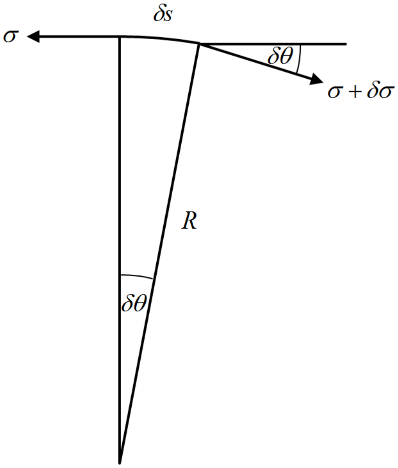

*Figure 4-3: Diagrammatic representation of the forces acting on an element of a two-dimensional curved surface.*

For the case of a static interface, Equation 4-26 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 4-27 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*.

### EXTERNAL FLUID INTERFACE

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 4-23 becomes:

$$\mathbf{n}_i \cdot \tau_1 = -p_{\mathrm{ext}}\mathbf{n}_i + \mathbf{f}_{st} \tag{4-28}$$

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, $p_{\mathrm{ext}}$, 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 4-22 can be dropped. Equation 4-24 is retained with $M_f$=0.

### *Wall Fluid Interface 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 Navier Slip boundary condition must be used on the walls. The forces acting on the contact point are applied to the model by the Wall-Fluid Interface node.

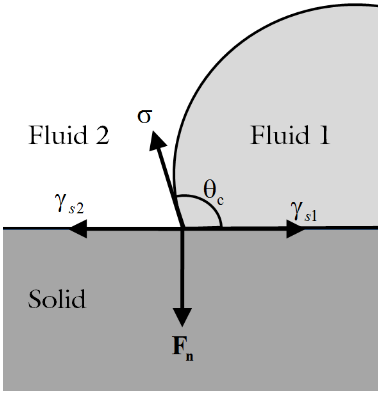

*Figure 4-4: Forces per unit length acting on a fluid-fluid interface at a three phase boundary with a solid wall. The surface tension force per unit length, σ, is balanced by a reaction force per unit length at the surface,* $\mathbf{F}_n$*, and by the forces generated by the surface energies of the two phases at the interface:* $\gamma_{s1}$ *and* $\gamma_{s2}$*.*

In equilibrium, the surface tension forces and the normal restoring force from the surface are in balance at a constant contact angle ($\theta_c$), as shown in Figure 4-4. This equilibrium is expressed by Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_c) + \gamma_{s1} = \gamma_{s2} \tag{4-29}$$

where σ is the surface tension force between the two fluids, $\gamma_{s1}$ is the surface energy density on the fluid 1—solid interface and $\gamma_{s2}$ is the surface energy density on the fluid 2—solid interface.

There is still debate in the literature as to precisely what occurs in non-equilibrium 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 towards 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, 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 wall-fluid interface 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 4-5.

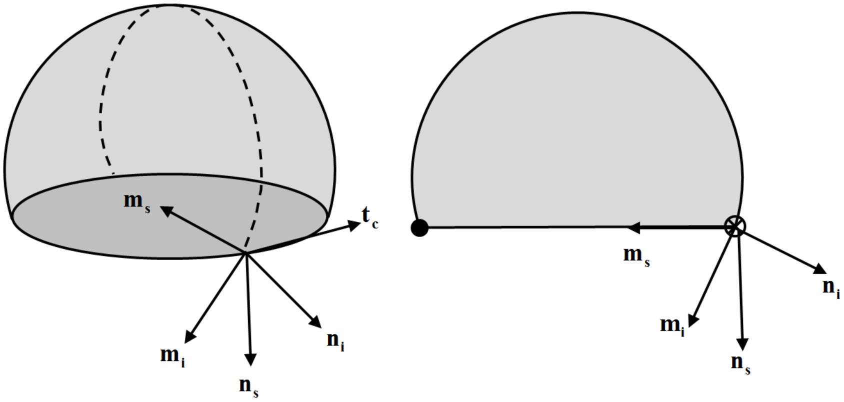

*Figure 4-5: Diagram showing normal and tangential vectors defined on the interface between two fluids and a solid surface in 3D (left) and 2D (right). The following vectors are defined:* $\mathbf{n}_i$*, the fluid-fluid interface unit normal;* $\mathbf{n}_s$*, the solid surface unit normal;* $\mathbf{t}_c$*, 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. Scardovell and S. Zalesk, “Direct Numerical Simulation of Free Surface and Interfacial Flow,” *Annu. Rev. Fluid Mech.*, vol. 31, pp. 567–60, 1999.

2. J. Gerbeau and T. Lelievre, “Generalized Navier Boundary Condition and Geometric Conservation Law for Surface Tension,” *Computer Methods In Applied Mechanics and Engineering*, vol. 198, pp. 644–656, 2009.

3. W. Ren and E. Weinan, “Boundary Conditions for the Moving Contact Line Problem,” *Physics of Fluids*, vol. 19, p. 022101, 2007.

4. W. Ren and D. Hu, “Continuum Models for the Contact Line Problem,” *Physics of Fluids*, vol. 22, p. 102103, 2010.

# 5

# Mathematics, Moving Interfaces

The Level Set and Phase Field Moving Interfaces are available under the **Mathematics>Moving Interface** branch ( ) when adding interfaces. See Modeling Microfluidic Fluid Flows to help you select which interface to use.

- The Level Set Interface
- The Phase Field Interface
- The Ternary Phase Field Interface
- Theory for the Level Set Interface
- Theory for the Phase Field Interface
- Theory for the Ternary Phase Field 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 since 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) and **Initial Values**. 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`.

### 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 Non-Conservative Form
- Domain, Boundary, and Pair Nodes for the Level Set Interface
- Theory for the Level Set Interface
- Theory for the Level Set and Phase Field Interfaces

## *Domain, Boundary, and Pair Nodes for the Level Set Interface*

The Level Set Interface has the following domain, boundary and pair nodes described.

- Initial Interface
- Initial Values
- Inlet
- Level Set Model
- No Flow
- Outlet[1]
- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Symmetry[1]

[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 2-3 for links to common sections and Table 2-4 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*

The **Level Set Model** node adds the following transport equation governing a level set function $\phi$

$$\frac{\partial\phi}{\partial t}+\mathbf{u}\cdot\nabla\phi = \gamma\nabla\cdot\left(\varepsilon\nabla\phi-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)$$

and 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** $\gamma$ (SI unit: m/s). The default is 1 m/s.

Enter a value or expression for the **Parameter controlling interface thickness** $e_{\mathrm{ls}}$ (SI unit: m). The default expression is `ls.hmax/2`, which means that the value is half of the maximum mesh element size in the region through which the interface passes.

### 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.

## *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 **Domain Initially** as one of the following:

- **Specify level set function explicitly**
- **Fluid 1 ($\phi$ = 0)**
- **Fluid 2 ($\phi$ = 1)**

> If the **Phase Initialization** () study step is being used, for the initialization to work it is crucial that there are two Initial Values nodes and one Initial Interface node. The Initial Values nodes should specify the **Domain Intially** as **Fluid 1** and **Fluid 2** respectively. The Initial Interface node should include all interior boundaries that defines the initial position of the fluid-fluid interface.. If the selection of the **Initial interface** node is empty, the initialization fails.
>
> See Initializing the Level Set Function.

## *Inlet*

The **Inlet** node adds a boundary condition for inlets (inflow boundaries).

### SETTINGS

Specify **Level Set Condition** as one of the following:

- **Fluid 1 (**$\phi = 0$**)**
- **Fluid 2 (**$\phi = 1$**)**
- **Specify level set function explicitly**

When choose specify level set function explicitly, a value of the level set function $\phi$ must be specified. The value must be in the range from 0 to 1, and the default is 0.

## *Initial Interface*

The **Initial Interface** node defines the boundary as the initial position of the interface $\phi = 0$.

If the **Transient with Initialization** ( ) study is being used, for the initialization to work it is crucial that there are two Initial Values nodes and one Initial Interface node. One of the Initial Values nodes should use **Domain initially: Inside interface** and the other **Domain initially: Outside interface**. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the **Initial interface** node is empty, the initialization fails.

See Initializing the Level Set Function.

## *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.

# The Phase Field Interface

The **Phase Field (pf)** interface ( ), found under the **Mathematics>Moving Interface** branch ( ) when adding a physics interface, is used to track moving interfaces by solving two transport equations, one for the phase field variable, $\phi$, and one for the mixing energy density, $\psi$. 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) and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **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 `pf`.

### DEPENDENT VARIABLES

This interface defines the dependent variables (fields) **Phase field variable** $\phi$ and **Phase field help variable** $\psi$. If required, edit the name, but dependent variables must be unique within a model.

- Conservative and Non-Conservative Forms
- Domain, Boundary, and Pair Nodes for the Phase Field Interface
- Theory for the Phase Field Interface

## *Domain, Boundary, and Pair Nodes for the Phase Field Interface*

The Phase Field 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.

- Initial Interface
- Initial Values
- Inlet
- Outlet[1]
- Periodic Condition (see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*)
- Phase Field Model
- Symmetry[1]
- Wetted Wall

[1] Described for the Laminar Flow interface.

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 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** $\sigma$ (SI unit: N/m).

- **Parameter controlling interface thickness** $e_{pf}$ (SI unit: m). The default expression is `pf.hmax/2`, which means that the value is half of the maximum mesh element size in the region through which the interface passes.
- **Mobility tuning parameter** $\chi$ (SI unit: m·s/kg). The default is 1 m·s/kg, which is a good starting point for most models. This parameter determines the time scale of the Cahn-Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface.

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💡 Keep the $\chi$ 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: 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 $\phi$ and then enter it into the $\phi$**-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

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## *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 **Domain Initially** as one of the following:

- **Specify phase field function explicitly**
- **Fluid 1 (**$\phi$ = -1**)**
- **Fluid 2 (**$\phi$ = 1**)**

> !
>
> If the **Phase Initialization** ( ) study step is being used, for the initialization to work it is crucial that there are two Initial Values nodes and one Initial Interface node. The Initial Values nodes should specify the **Domain Initially** as **Fluid 1** and **Fluid 2** respectively. The Initial Interface node should include all interior boundaries that defines the initial position of the fluid-fluid interface. If the selection of the **Initial interface** node is empty, the initialization fails.

## *Inlet*

The **Inlet** feature node adds a boundary condition for inlets (inflow boundaries).

### SETTINGS

Specify **Phase field Condition** as one of the following:

- **Fluid 1 (**$\phi$ = -1**)**
- **Fluid 2 (**$\phi$ = 1**)**
- **Specify phase field function explicitly**

When choose specify phase field function explicitly, a value of the phase field function $\phi$ must be specified. The value must be in the range from -1 to 1, and the default is 1.

## *Initial Interface*

The **Initial Interface** node defines the boundary as the initial position of the interface $\phi = 0$.

!

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 and one **Initial Interface** node. One of the Initial Values nodes is set to `phipf = 1` and the other to `phipf = -1`. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the Initial Interface node is empty, the initialization fails.

## *Wetted Wall*

The **Wetted Wall** node is the default boundary condition representing wetted walls. Along a wetted wall the contact angle for the fluid, $\theta_w$, 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

$$\mathbf{n}\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi = 0$$

### WETTED WALL

Enter a value or expression for the **Contact angle** $\theta_w$. The default value is $\pi/2$ rad.

# 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, $\phi_A$ and $\phi_B$ , and two equations for the corresponding generalized chemical potentials, $\eta_A$ and $\eta_B$. 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 Ternary Phase Field interface

## Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface

The Ternary Phase Field 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 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.

### PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- **Parameter controlling interface thickness** $\varepsilon$. The default expression applied is `terpf.hmax*sqrt(2)`, which means that the thickness is related to the maximum mesh element size in the domain. If the element size in the regions passed by the interfaces is known beforehand, it is recommended to apply a value of $\varepsilon$ in that order.

- **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 $1 \cdot 10^{-4}$ $\mathrm{m}^3 \cdot \mathrm{s/kg}$, which is a good starting point for most models.
- **Additional free bulk energy** $\Lambda$. When needed add an a user defined expression of 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 (for example, **Water/Air**, **Glycerol/Air**, and so forth).
- For **User defined**, enter a value or expression for the surface tension coefficient

#### CONVECTION

Enter values or expressions for the components ($u$, $v$, and $w$ in 3D, for example) of the **Velocity field** $\mathbf{u}$. 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*

This condition should be used on boundaries which 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** $\theta_\alpha$.
- The **Contact angle of interface from phase B to phase C** $\theta_\beta$.
- The **Contact angle of interface from phase A to phase B** $\theta_\gamma$.

The definition of the contact angles with respect to the wall are shown in the figure below

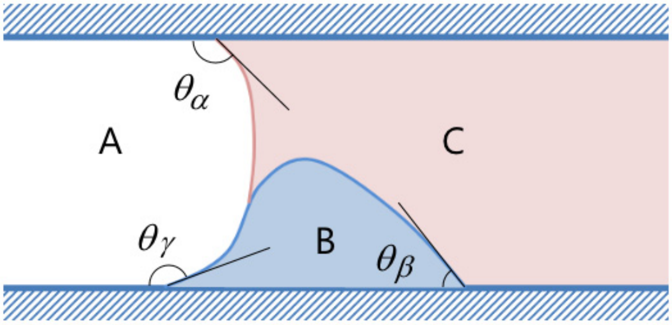

*Figure 5-1: Definitions of the contact angels in the Wetted Wall feature of the Ternary Phase Field interface.*

# 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 Non-Conservative 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 5-2 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 $\phi$. In COMSOL Multiphysics, $\phi$ 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 $\phi$. Figure 5-3 shows the level set representation of the interface in Figure 5-2.

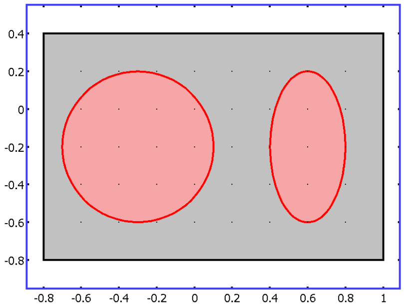

*Figure 5-2: An example of two domains divided by an interface. In this case, one of the domains consists of two parts.* Figure 5-3 *shows the corresponding level set representation.*

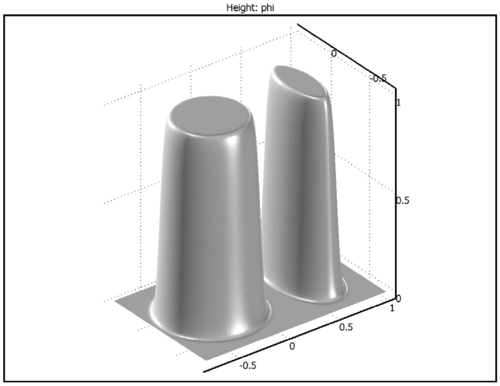

*Figure 5-3: A surface plot of the level set function corresponding to* Figure 5-2.

The physics interface solves Equation 5-1 in order to move the interface with the velocity field **u**:

$$\frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = \gamma\nabla \cdot \left(\varepsilon\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right) \tag{5-1}$$

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, $\varepsilon$, determines the thickness of the region where $\phi$ varies smoothly from zero to one and is typically of the same order as the size of the elements of the mesh. By default, $\varepsilon$ is constant within each domain and equals the largest value of the mesh size, $h$, within the domain. The parameter $\gamma$ determines the amount of reinitialization or stabilization of the level set function. It needs to be tuned for each specific problem. If $\gamma$ is too small, the thickness of the interface might not remain constant and oscillations in $\phi$ can appear because of numerical instabilities. On the other hand, if $\gamma$ is too large the interface moves incorrectly. A suitable value for $\gamma$ is the maximum magnitude of the velocity field $\mathbf{u}$.

## *Conservative and Non-Conservative Form*

If the velocity is divergence free, that is, if

$$\nabla \cdot \mathbf{u} = 0 \tag{5-2}$$

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, switch to the conservative form

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \gamma \nabla \cdot \left( \varepsilon \nabla \phi - \phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|} \right) \tag{5-3}$$

in Settings window for The Level Set Interface.

Using the conservative level set form, exact numerical conservation of the integral of $\phi$ is obtained. However, the non-conservative form is better suited for numerical calculations and usually converges more easily. The non-conservative form, which is the default form, only conserves the integral of the level set function approximately, but this is sufficient for most applications.

## *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, $D_{\mathrm{wi}}$. 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 outside the interface and

$$\phi_0 = \frac{1}{1+e^{D_{\mathrm{wi}}/\varepsilon}}$$

in domains initially inside the interface. Here, inside refers to domains where $\phi < 0.5$ and outside refers to domains where $\phi > 0.5$.

! For the initialization to work it is crucial that there are two **Initial Values** nodes and one **Initial Interface** node. One of the Initial Values nodes should use **Domain initially: Inside interface** and the other **Domain initially: Outside interface**. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the Initial interface node is empty, the initialization fails.

- The Level Set Interface
- Studies and Solvers and Transient 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

$$\mathbf{n} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi = 0{,}5} \tag{5-4}$$

The curvature is defined as

$$\kappa = -\nabla\cdot\mathbf{n}|_{\phi = 0{,}5} \tag{5-5}$$

These variables are available in the physics interface as the interface normal and mean curvature.

It is only possible to compute the curvature explicitly when using second-order or higher-order elements.

### *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 Interface

The Phase Field Interface theory is described in this section:

- About the Phase Field Method
- The Equations for the Phase Field Method
- Conservative and Non-Conservative Forms
- Additional Sources of Free Energy
- Initializing the Phase Field Function
- Variables and Expressions
- Reference for the Phase Field 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, $\phi$. 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 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, $\phi$:

$$F(\phi, \nabla\phi, T) = \int\left(\frac{1}{2}\varepsilon^2|\nabla\phi|^2 + f(\phi, T)\right)dV = \int f_{\mathrm{tot}}dV$$

where ε is a measure of the interface thickness. Equation 5-6 describes the evolution of the phase field parameter:

$$\frac{\partial\phi}{\partial t} + (\mathbf{u}\cdot\nabla)\phi = \nabla\cdot\gamma\nabla\left(\frac{\partial f_{\mathrm{tot}}}{\partial\phi} - \nabla\cdot\frac{\partial f_{\mathrm{tot}}}{\partial\nabla\phi}\right) \tag{5-6}$$

where $f_{\mathrm{tot}}$ (SI unit: $\mathrm{J/m^3}$) 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 5-6 aims to minimize the total free energy with a relaxation time controlled by the mobility $\gamma$ (SI unit: $\mathrm{m^3\cdot s/kg}$).

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:

$$f_{\mathrm{mix}}(\phi, \nabla\phi) = \frac{1}{2}\lambda|\nabla\phi|^2 + \frac{\lambda}{4\varepsilon^2}(\phi^2 - 1)^2$$

where $\phi$ 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 $\lambda$ (SI unit: N) is the mixing energy density and $\varepsilon$ (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, $\sigma$ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon} \tag{5-7}$$

The PDE governing the phase field variable is the Cahn-Hilliard equation:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\gamma\nabla G \tag{5-8}$$

where $G$ (SI unit: Pa) is the chemical potential and $\gamma$ (SI unit: $\mathrm{m^3\cdot s/kg}$) 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:

$$G = \lambda\left[-\nabla^2\phi + \frac{\phi(\phi^2-1)}{\varepsilon^2}\right] \tag{5-9}$$

The Cahn-Hilliard equation forces $\phi$ to take a value of 1 or −1 except in a very thin region on the fluid-fluid interface. The Phase Field interface breaks Equation 5-8 up into two second-order PDEs:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi \tag{5-10}$$

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2-1)\phi \tag{5-11}$$

## Conservative and Non-Conservative Forms

If the velocity field is divergence free, use the conservative formulation:

$$\frac{\partial\phi}{\partial t} + \nabla\cdot\mathbf{u}\phi = \nabla\cdot\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi$$

Using the conservative phase field form, exact numerical conservation of the integral of $\phi$ is obtained. However, the non-conservative form is better suited for numerical calculations and usually converges more easily. The non-conservative form, which is the default form, only conserves the integral of the phase field function approximately, but this is sufficient for most applications.

## 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 5-11:

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2-1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f}{\partial\phi} \tag{5-12}$$

where *f* is a user-defined free energy (SI unit: $J/m^3$).

The expression for the external free energy must be manually differentiated with respect to $\phi$ 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, $D_{\mathrm{wi}}$. The Time Dependent step then uses the initial condition for the phase field function according to the following 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 5-10 and Equation 5-11 for a straight, non-moving 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 and one **Initial Interface** node. One of the Initial Values nodes is set to *phipf* = 1 and the other to *phipf* = -1. The Initial Interface node should have all interior boundaries where the interface is initially present as selection. If the selection of the Initial Interface node is empty, the initialization fails.

Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

### *Variables and Expressions*

Unlike the level set method, the phase field method does not require expressions for the unit normal to the interface or smoothed delta functions, so they are not available for analysis. Variables that are defined are the chemical potential, which can be rewritten in terms of the dependent variable $\psi$,

$$G = \frac{\lambda\psi}{\varepsilon^2}$$

and the surface tension force $\mathbf{F} = G\nabla\phi$ .

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 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 Ternary Phase Field interface

The Ternary Phase Field Interface theory is described in this section:

- About the Phase Field Method
- The Equations for the Phase Field Method
- Reference for the Phase Field 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. 1. 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 $\phi$ which takes values between 0 and 1. The phase field variables satisfies the constraint

$$\sum_{i = \mathrm{A}, B, C} \phi_i = 0 \tag{5-13}$$

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:

$$\begin{aligned} F = {} & \sigma_{AB}\phi_A^2\phi_B^2 + \sigma_{AC}\phi_A^2\phi_C^2 + \sigma_{BC}\phi_B^2\phi_C^2 + \\ & \phi_A\phi_B\phi_C(\Sigma_A\phi_A + \Sigma_B\phi_B + \Sigma_C\phi_C) + \Lambda\phi_A^2\phi_B^2\phi_C^2 \end{aligned} \tag{5-14}$$

Here the $\sigma_{ij}$ denotes the surface tension coefficient of the interface separating phase $i$ and $j$, and the capillary parameters $\Sigma_i$ are defined as

$$\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk} \tag{5-15}$$

and $\Lambda$ is a function or parameter specifying the additional free bulk energy. By default $\Lambda$ is zero. In this case it can be seen that the free energy in Equation 5-14 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

$$\begin{aligned} \frac{\partial\phi_i}{\partial t} + \frac{\partial u_j\phi_i}{\partial x_j} &= \frac{\partial}{\partial x_j}\left(\frac{M_0}{\Sigma_i}\frac{\partial\eta_i}{\partial x_j}\right) \\ \eta_i &= \frac{4\Sigma_{\mathrm{T}}}{\varepsilon}\sum_{j \neq i}\left(\frac{1}{\Sigma_j}\left(\frac{\partial F}{\partial\phi_i} - \frac{\partial F}{\partial\phi_j}\right)\right) - \frac{3}{4}\varepsilon\Sigma_j\frac{\partial}{\partial x_j}\left(\frac{\partial\eta_i}{\partial x_j}\right) \end{aligned} \tag{5-16}$$

It can be noted that the Cahn-Hilliard equation is originally a 4th-order PDE. In COMSOL this is split up into two second order PDEs by introducing an additional dependent variable, the generalized potential $\eta$, one for each phase. In order to satisfy Equation 5-14, two sets of the equations shown in Equation 5-16 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 5-14.

In Equation 5-16 $\varepsilon$ (SI unit: 1/m) is a parameter controlling the interface thickness, $M_0$ (SI unit: $\mathrm{m}^3$/s) is a molecular mobility parameter, and the parameter $\Sigma_{\mathrm{T}}$ is defined as

$$\frac{3}{\Sigma_{\mathrm{T}}} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \tag{5-17}$$

## *Reference for the Ternary 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.

# 6

# Porous Media Flow Interfaces

This chapter discusses the physics interfaces found under the **Fluid Flow>Porous Media and Subsurface Flow** branch ( ). See Modeling Microfluidic Fluid Flows to help you select which physics interface to use.

In this chapter:

- The Darcy's Law Interface
- The Brinkman Equations Interface
- The Free 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 Interface

# 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 Fluid and Matrix Properties node, which provides an interface for defining the fluid material along with the porous medium properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder**— **Fluid 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 **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** $p_{\mathrm{ref}}$ (SI unit: Pa). The default value is `1[atm]`.

#### 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.

### DISCRETIZATION

To display this section, click the **Show** button ( ) and select **Discretization.**

The **Compute boundary fluxes** check box 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 check box is cleared, COMSOL 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** check box is available if the previous check box 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.

- 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*

## *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 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.

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 2-3 for links to common sections and Table 2-4 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

- Fluid and Matrix Properties
- Mass Source
- Initial Values

### BOUNDARY, EDGE, AND POINT

The following nodes (listed in alphabetical order) are available on exterior boundaries:

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.

## *Fluid and Matrix Properties*

The **Fluid and Matrix Properties** node adds the equations for Darcy's law, Equation 6-1 and Equation 6-2(excluding any mass sources), and contains settings for the fluid properties and the porous matrix properties such as the effective porosity.

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\nabla\cdot(\rho\mathbf{u}) = Q_{\mathrm{m}} \tag{6-1}$$

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{6-2}$$

### FLUID PROPERTIES

Select the **Fluid material** to use for the fluid properties. Select **Domain material** (the default) to use the material defined for the domain. Select another material to use that material's properties for the fluid.

#### *Density*

The default **Density** $\rho$ (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$^3$.
- 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.

#### *Dynamic Viscosity*

Select a **Dynamic viscosity** $\mu$ (SI unit: Pa·s). The default uses values **From material** as defined by the **Fluid material** selected. For **User defined** the default is 0 Pa·s.

### MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** from the **Porous material** list (the default) to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** $\varepsilon_{\mathrm{p}}$ (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.

The default **Permeability** $\kappa$(SI unit: $\mathrm{m}^2$) uses the value **From material**, as defined by the **Porous material** selected. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to define a tensor value and enter another value or expression in the field or matrix.

## *Mass Source*

The **Mass Source** node adds a mass source $Q_\mathrm{m}$, which appears on the right-hand side of the Darcy's Law equation (Equation 6-8, the equation for porosity).

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho\mathbf{u}) = Q_\mathrm{m} \tag{6-3}$$

### MASS SOURCE

Enter a value or expression for the **Mass source** $Q_\mathrm{m}$ (SI unit: $\mathrm{kg/(m^3{\cdot}s)}$). The default is 0 $\mathrm{kg/(m^3{\cdot}s)}$.

## *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.

### INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** $p$ (SI unit: Pa). The default value is 0 Pa.

## *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.

### 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).

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ☰ ) and select **Advanced Physics Options**.

## *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:

$$\mathbf{n}\cdot\rho\frac{\kappa}{\mu}\nabla p = N_0$$

where $N_0$ is a value or expression for the specified inward (or outward) Darcy flux.

### 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)), **Edges** (SI unit: kg/(m·s), and **Points** (SI unit: kg/s)).

## *Inlet*

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary:

$$\mathbf{n}\cdot\rho\frac{\kappa}{\mu}\nabla p = \rho U_0$$

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.

### 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. A negative value represents an outflow velocity.

## *Symmetry*

The **Symmetry** node describes a symmetry boundary. The following condition implements the symmetry condition on an axis or a flow divide:

$$\mathbf{n}\cdot\frac{\kappa}{\mu}\nabla p = 0$$

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.

## No Flow

The **No Flow** node is the default boundary condition stating that there is no flow across impervious boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho\frac{\kappa}{\mu}\nabla p = 0$$

where $\mathbf{n}$ is the vector normal to the boundary.

## 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, $\rho$ is the fluid density, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the Darcy's velocities in the adjacent domains (as defined in Equation 6-7) and $N_0$ is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{6-4}$$

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.

## Outlet

The **Outlet** node adds a boundary condition for the outflow (or inflow) perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = \rho U_0$$

where $U_0$ is a specified value or expression for the outward (or inward) Darcy velocity. A positive value of the velocity $U_0$ corresponds to flow out of the model domain whereas a negative value represents an inflow.

### OUTLET

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.

# 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 Fluid and Matrix Properties feature, which adds the Brinkman equations and provides an interface 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**—**Fluid and Matrix Properties**, **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

$$\frac{1}{\varepsilon_{\mathrm{p}}}\left\{\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}$$

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections such as **Discretization**, **Consistent Stabilization**, and **Inconsistent Stabilization**, and **Advanced Settings** sections, 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, select **Compressible flow (Ma<0.3)** from the **Compressibility** list if there are small variations in the density, typically dependent on the temperature (non-isothermal flow). For compressible flow modeled with the Brinkman Equations interface, the Mach number must be below 0.3.

#### *Neglect Inertial Term (Stokes-Brinkman Flow)*

The **Neglect inertial term (Stokes-Brinkman)** check box is selected by default to model flow at very low Reynolds numbers for which the inertial term can be neglected in the Brinkman equations. This results in the linear Stokes-Brinkman equations.

#### *Enable porous media domains*

The **Enable porous media domains** check box is selected by default to solve Brinkman equations in porous domains.

#### *Reference Pressure Level*

Enter a **Reference pressure level** $p_{\mathrm{ref}}$ (SI unit: Pa). The default value is `1[atm]`.

### 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** button ( 👁 ) and select **Advanced Physics Options**. 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.

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- 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
- Discontinuous Galerkin Formulation

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## *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).

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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.

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These nodes are described in this section:

- Fluid and Matrix Properties
- Forchheimer Drag
- Initial Values
- Mass Source
- Volume Force
- Fluid Properties

The following nodes(listed in alphabetical order) are described for the Laminar Flow interface :

- Flow Continuity
- InletLine Mass Source
- Boundary Stress
- Outlet
- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point ConstraintSymmetry
- Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 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 and Matrix Properties*

The **Fluid and Matrix Properties** node adds the Brinkman equations: Equation 6-10 and Equation 6-11 (excluding any mass sources), and provides an interface for defining the properties of the fluid material and the porous matrix The Forchheimer Drag subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

Both the default **Density** $\rho$ (SI unit: kg/m$^3$) and **Dynamic viscosity** $\mu$ (SI unit: Pa·s) use values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. In this case, the default is 0 kg/m$^3$ for the density and 0 Pa·s for the dynamic viscosity. 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. Non-Newtonian fluids have a viscosity that is shear-rate dependent. Examples of non-Newtonian fluids include yoghurt, paper pulp, and polymer suspensions.

### POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** (the material defined for the domain) for the porous matrix. Select another material as needed.

Both the default **Porosity** $\varepsilon_p$ (a dimensionless number between 0 and 1) and **Permeability** $\kappa$ (SI unit: $m^2$) use values **From material** as defined by the **Porous material** selection. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the characteristics of the permeability, and enter another value or expression. The components of a permeability in the case that it is a tensor ($\kappa_{xx}$, $\kappa_{yy}$, and so on, representing an anisotropic permeability) are available as `br.kappaxx`, `br.kappayy`, and so on (using the default name `br`).

## *Forchheimer Drag*

The **Forchheimer Drag** subnode is available from the context menu (right-click the Fluid and Matrix Properties parent node) or from the **Physics** toolbar, **Attributes** menu. While the drag of the fluid on the porous matrix in the basic Brinkman equations is proportional to the flow velocity, (Darcy's law drag), the Forchheimer drag is proportional to the square of the fluid velocity. The latter 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.

### FORCHHEIMER DRAG

Enter a value for the **Forchheimer coefficient** $\beta_F$ (SI unit: $kg/m^4$). The default is $0\ kg/m^4$.

## *Mass Source*

The **Mass Source** node adds a mass source (or mass sink) $Q_{br}$ to the right-hand side of the continuity equation: Equation 6-10. 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.

$$\frac{\partial}{\partial t}(\varepsilon_p\rho) + \nabla \cdot (\rho\mathbf{u}) = Q_{br} \qquad (6\text{-}5)$$

### DOMAIN SELECTION

Only Porous Matrix domains are available.

#### MASS SOURCE

Enter a value or expression for the **Source term** $Q_{\mathrm{br}}$ (SI unit: kg/(m$^3$·s)). The default is 0 kg/(m$^3$·s).

## *Volume Force*

Use the **Volume Force** node to specify the force $\mathbf{F}$ on the right-hand side of Equation 6-11. It then acts on each fluid element in the specified domains. A common application is to include gravity effects.

$$\frac{\rho}{\varepsilon_{\mathrm{p}}}\left(\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\frac{\mathbf{u}}{\varepsilon_{\mathrm{p}}}\right) = \\ -\nabla p+\nabla\cdot\left[\frac{1}{\varepsilon_{\mathrm{p}}}\left\{\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}\right]-\left(\kappa^{-1}\mu+\frac{Q_{\mathrm{br}}}{\varepsilon_{\mathrm{p}}^2}\right)\mathbf{u}+\mathbf{F} \tag{6-6}$$

#### VOLUME FORCE

Enter the components of **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 the **Pressure** $p$ (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

## *Fluid Properties*

The **Fluid Properties** node adds the momentum and continuity equations to solve for free flow in non-porous 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 and/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 $p$+$p_{\mathrm{ref}}$ where $p$ is the dependent pressure variable from the Navier-Stokes equations, and $p_{\mathrm{ref}}$ is from the user input defined at the physics interface level. When $p_{\mathrm{ref}}$ is non zero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, $p_{\mathrm{ref}}$ 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** $\mu$ 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.

# The Free and Porous Media Flow Interface

The **Free and Porous Media Flow (fp)** 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 where free flow is connected to porous media. The Free and Porous Media Flow 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 Matrix Properties** 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** 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 **Compressible flow (Ma<0.3)** from the **Compressibility** list, to account for small variations in the density, typically dependent on the temperature (non-isothermal flow). For compressible flow modeled with this physics interface, the Mach number must be below 0.3.

#### *Neglect Inertial Term*

Select the **Neglect inertial term in free flow (Stokes flow)** check box if the inertial forces are small compared to the viscous forces. This is typical for creeping flow, where $\mathrm{Re} \ll 1$.

Select the **Neglect inertial term in porous media flow (Stokes-Brinkman)** check box to model flow at very low Reynolds numbers in the porous media, for which the inertial term in the Brinkman equations can be neglected. The physics interface then solves the linear Stokes-Brinkman equations.

#### *Reference Pressure Level*

Enter a **Reference pressure level** $p_{\mathrm{ref}}$ (SI unit: Pa). The default value is `1[atm]`.

### 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 Interface
- Theory for the Free and Porous Media Flow Interface

## *Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow Interface*

The Free and Porous Media Flow 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
- Forchheimer Drag
- Initial Values
- Mass Source
- Microfluidic Wall Conditions
- Porous Matrix Properties
- Volume Force
- Wall

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 2-3 for links to common sections and Table 2-4 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** $\rho$ (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** $\mu$ (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 Matrix Properties*

Use the **Porous Matrix Properties** node to define which domains contain porous material and to define the porous matrix properties, such as the porosity and permeability in these domains. The Forchheimer Drag subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### DOMAIN SELECTION

Choose domains from the **Selection** list, to solve for porous media flow governed by the Brinkman equations. In the domains not selected, the Free and Porous Media Flow interface solves for laminar flow governed by the Navier-Stokes (or Stokes) equations.

### POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** (the material defined for the domain) for the porous matrix. Select another material as needed.

*Porosity*

The default **Porosity** $\varepsilon_\mathrm{p}$ (a dimensionless number between 0 and 1) uses values **From material** as defined by the **Porous material** selection. For **User defined** enter another value or expression. The default is 0.

*Permeability*

The default **Permeability** $\kappa_\mathrm{br}$ (SI unit: $\mathrm{m}^2$) uses values **From material** as defined by the **Porous material** selection. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** from the list and then enter other values or expressions. The components of a permeability in the case that it is a tensor ($\kappa_{xx}$, $\kappa_{yy}$, and so on, representing an anisotropic permeability) are available as `fp.kappaxx`, `fp.kappayy`, and so on (using the default name `fp`). The default is 0 $\mathrm{m}^2$.

*Source Term*

Enter a value or expression for an optional mass source (or sink) **Source term** $Q_\mathrm{br}$ (SI unit: $\mathrm{kg/(m^3{\cdot}s)}$). This term accounts for mass deposit and mass creation within domains. The physics interface assumes that the mass exchange occurs at zero velocity.

## *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 the Porous Matrix

Properties node is active for the domain. Use it, for example, to incorporate the effects of gravity in a model.

### VOLUME FORCE

Enter the components of the **Volume force** $\mathbf{F}$ (SI unit: N/m$^3$).

## *Forchheimer Drag*

The **Forchheimer Drag** subnode is available from the context menu (right-click the Porous Matrix Properties parent node) or from the **Physics** toolbar, **Attributes** menu. It can be used on the domain selection that corresponds to the porous medium. For the Brinkman equations the drag of the fluid on the porous matrix is proportional to the flow velocity, in the same way as for Darcy's law. Add a Forchheimer drag, proportional to the square of the fluid velocity, as needed.

### FORCHHEIMER DRAG

Enter a value for the **Forchheimer coefficient** $\beta_{\mathrm{F}}$ (SI unit: kg/m$^4$).

## *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.

## *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** $\mathbf{u}_{\mathrm{w}}$ (SI unit: m/s).

#### Use Viscous Slip

Select the **Use viscous slip** check box 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) $a_v$ (dimensionless) (the default is 0.9) and the **Mean free path** $\lambda$ (SI unit: m) (the default is 1e-6 m).

#### Use Thermal Creep

Select the **Use thermal creep** check box to activate the thermal creep component of the boundary condition. Enter the fluid's **Temperature** $T$ (SI unit: K) and the **Thermal slip coefficient** $\sigma_T$. 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
- Sliding Wall
- Moving Wall
- 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.

### *Sliding Wall*

The **Sliding wall** boundary condition 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** $\mathbf{u}_\mathrm{w}$ 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** $U_\mathrm{w}$ should be specified in 2D.
- For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the **Velocity of moving wall**, $\varphi$ **component** $v_\mathrm{w}$ may also be specified.

### *Moving Wall*

For an arbitrary wall movement, the condition $\mathbf{u} = \mathbf{u}_\mathrm{w}$ may be prescribed. In this case, the components of the **Velocity of moving wall** $\mathbf{u}_\mathrm{w}$ should be specified.

Specifying this boundary condition 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.

### *Leaking Wall*

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_\mathrm{l}$ through a perforated wall. The components of the **Fluid velocity** $\mathbf{u}_\mathrm{l}$ 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
- Moving Mesh Interface in the *COMSOL Multiphysics Reference Manual*

# Theory for the Darcy's Law Interface

The Darcy's Law Interface theory is described in this section.

In a porous medium, the global transport of momentum by shear stresses in the fluid is often negligible: the pore walls impede momentum transport between fluid occupying different pores. In most applications, a detailed description of the resolution of every pore is not practical. 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 provides a complete mathematical model suitable for a variety of applications involving porous media flows when the pressure gradient is the major driving force.

## *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:

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{6-7}$$

In this equation, $\kappa$ (SI unit: $\mathrm{m}^2$) denotes the permeability of the porous medium, $\mu$ (SI unit: kg/(m·s)) the dynamic viscosity of the fluid, $p$ (SI unit: Pa) the pressure, and $\mathbf{u}$ (SI unit: m/s) the Darcy velocity. The Darcy's Law interface combines Darcy's law with the continuity equation:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla\cdot(\rho\mathbf{u}) = Q_\mathrm{m} \tag{6-8}$$

In the above equation, $\rho$ (SI unit: $\mathrm{kg/m^3}$) is the density of the fluid, $\varepsilon$ (dimensionless) is the porosity, and $Q_\mathrm{m}$ (SI unit: $\mathrm{kg/(m^3{\cdot}s)}$) is a mass source term. 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.

If the Darcy's Law interface is coupled to an energy balance, then the fluid density can be a function of the temperature, pressure, and composition (for mixture flows). For gas flows in porous media, the relation is given by the ideal gas law:

$$\rho = \frac{pM}{RT} \tag{6-9}$$

where $R$= 8.314 J/(mol·K) is the universal gas constant, $M$ (SI unit: kg/mol) is the molecular weight of the gas, and $T$ (SI unit: K) is the temperature.

# 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 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.

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The Free and Porous Media Flow Interface

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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:

$$\frac{\partial}{\partial t}(\varepsilon_p\rho) + \nabla\cdot(\rho\mathbf{u}) = Q_{\mathrm{br}} \tag{6-10}$$

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) =$$

$$-\nabla p + \nabla\cdot\left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_{\mathrm{br}}}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F} \tag{6-11}$$

In these equations:

- $\mu$ (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- $\mathbf{u}$ (SI unit: m/s) is the velocity vector
- $\rho$ (SI unit: kg/m$^3$) is the density of the fluid
- $p$ (SI unit: Pa) is the pressure
- $\varepsilon_p$ is the porosity
- $\kappa$ (SI unit: m$^2$) is the permeability tensor of the porous medium, and
- $Q_{\mathrm{br}}$ (SI unit: kg/(m$^3$·s)) is a mass source or mass 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-Brinkman) check box is selected, the term $(\mathbf{u}\cdot\nabla)(\mathbf{u}/\varepsilon_p)$ on the left-hand side of Equation 6-11 is disabled.

The mass source, $Q_{\mathrm{br}}$, accounts for mass deposit and mass creation within the domains. The mass exchange is assumed to occur at zero velocity.

The Forchheimer drag option, $\beta_F$ (SI unit: kg/m$^4$), adds a viscous force proportional to the square of the fluid velocity, $\mathbf{F}_F = -\beta_F|\mathbf{u}|\mathbf{u}$, to the right-hand side of Equation 6-11.

In case of a flow with variable density, Equation 6-10 and Equation 6-11 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

$$\frac{\partial}{\partial t}(\varepsilon_\mathrm{p}\rho) + \mathbf{u}\cdot\nabla\rho = 0$$

and the continuity equation (Equation 6-10) reduces to

$$\rho\nabla\cdot\mathbf{u} = Q_\mathrm{br}$$

## *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. of Fluid Mechanics*, vol. 550, pp. 149–173, 2006.

# Theory for the Free and Porous Media Flow Interface

The Free and Porous Media Flow 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 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.

# 7

# Rarefied Flow Interface

This chapter describes the physics interface available to model the flow of rarefied gases. The physics interface is found under the **Fluid Flow>Rarefied Flow** branch ( ). See Modeling Microfluidic Fluid Flows to help select the physics interface to use.

- The Slip Flow Interface
- Theory for the Slip Flow Interface

# The Slip Flow Interface

The **Slip Flow (slpf)** interface ( ), found under the **Rarefied Flow** branch ( ) when adding a physics interface, is used to model thermal and isothermal flows within the slip flow regime. In the slip flow regime, the Navier-Stokes equations can be used to model the flow of the gas, except within a thin layer of rarefied gas adjacent to the walls (known as the Knudsen layer). The effect of the Knudsen layer on the continuum part of the flow can be modeled by means of modified boundary conditions for the Navier Stokes equations. Thermal effects are also important in this regime, with effects such as thermal creep or transpiration often playing a significant role. For this reason the Slip Flow interface includes the heat flow equations. Typically slip flow applies at Knudsen numbers between 0.01 and 0.1.

When this physics interface is added, these default nodes are also added to the **Model Builder**: **Fluid**, **External Slip 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 **Slip 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 `slpf`.

### PHYSICAL MODEL

Select the **Neglect inertial term (Stokes flow)** check box to model flow at very low Reynolds numbers where the inertial term in the Navier-Stokes equations can be neglected. When this option is checked COMSOL Multiphysics solves the linear Stokes equations for the fluid flow. The *Stokes flow* or *creeping flow* regime frequently applies in microfluidic devices, where the flow length scales are very small. Enter a **Reference pressure level** $p_{\mathrm{ref}}$. The default value is `1[atm]`.

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If you have the Heat Transfer Module, additional check boxes are available. See the *Heat Transfer Module User's Guide for information*.

---

#### DEPENDENT VARIABLES

This physics interface defines these dependent variables (fields):

- **Temperature** T (SI unit: K)
- **Velocity field** u (SI unit: m/s)
- **Pressure** p (SI unit: Pa)

For each of the dependent variables, the name can be changed in the corresponding field, but the name of fields and dependent variables must be unique within a 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. The **Default model** is **Fluid**.

Select the **Use pseudo time stepping for stationary equation form** check box 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** $CFL_{\mathrm{loc}}$.

By default the **Enable conversions between material and spatial frames** check box is selected.

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In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 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.

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- Domain, Boundary, Edge, Point, and Pair Nodes for the Slip Flow Interface
- Theory for the Slip Flow Interface

In the *COMSOL Multiphysics Reference Manual:*

- Pseudo Time Stepping for Laminar Flow Models
- Handling Frames in Heat Transfer

*Slip Flow Benchmark*: Application Library path **Microfluidics_Module/Rarefied_Flow/slip_flow_benchmark**

## *Domain, Boundary, Edge, Point, and Pair Nodes for the Slip Flow Interface*

The Slip Flow Interface 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.

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 boundaries that represent the symmetry axis.

These nodes are available and described in this section (listed in alphabetical order):

- Continuity
- External Slip Wall
- Fluid
- Initial Values
- Periodic Condition
- Slip Wall
- Symmetry

### HEAT TRANSFER IN FLUIDS SUBMENU

These nodes and one subnode are described for the Heat Transfer interface in the *COMSOL Multiphysics Reference Manual* (listed in alphabetical order):

- Boundary Heat Source
- Heat Flux
- Heat Source
- Solid
- Line Heat Source
- Outflow
- Change Thickness
- Point Heat Source
- Diffuse Surface
- Temperature
- Thermal Insulation
- Thin Layer
- Translational Motion

### LAMINAR FLOW SUBMENU

These nodes are described for the Laminar Flow interface in this guide (listed in alphabetical order):

- Boundary Stress
- Inlet
- Line Mass Source
- Open Boundary
- Outlet
- Point Mass Source
- Pressure Point Constraint
- Volume Force
- Wall

---

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 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.

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## *Fluid*

The **Fluid** node prescribes its domains to be a fluid by adding momentum and energy transport equations.

#### HEAT CONDUCTION, FLUID

The default uses the **Thermal conductivity** $k$ (SI unit: W/(m·K)) **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the characteristics of the thermal conductivity and enter another value or expression in the field or matrix.

> The thermal conductivity describes the relationship between the heat flux vector $\mathbf{q}$ and the temperature gradient $\nabla T$ as in $\mathbf{q} = -k\nabla T$ which is Fourier's law of heat conduction. Enter this quantity as power per length and temperature.

#### THERMODYNAMICS, FLUID

The **Fluid type** defaults to **Gas/Liquid**.

By default the **Density** $\rho$ (SI unit: kg/m$^3$), **Heat capacity at constant pressure** $C_\mathrm{p}$ (SI unit: J/(kg·K)), and **Ratio of specific heats** $\gamma$ (dimensionless) take values **From material**. For **User defined** to enter other values or expressions.

#### DYNAMIC VISCOSITY

The default **Dynamic viscosity** $\mu$ (SI unit: Pa·s) is taken **From material**. Or select **Non-Newtonian power law**, **Non-Newtonian Carreau model**, or **User defined**. For **User defined** it uses a built-in variable for the shear rate magnitude, `spf.sr`, which makes it possible to define arbitrary expressions of the dynamic viscosity.

## *External Slip Wall*

Use the **External Slip Wall** node to specify a wall with slip when the adjacent wall is external to the whole geometry. The wall temperature, wall velocity, and slip coefficients are specified.

#### SLIP WALL

Enter the components for the **Velocity of moving wall** $\mathbf{u}_\mathbf{w}$.

Enter a value or expression for the **Wall temperature** $T_\mathrm{w}$. The default is 293.15 K.

Select the **Slip coefficients**: **Maxwell's model** (the default) or **User defined**.

##### *Maxwell's Model*

For **Maxwell's Model** enter values or expressions for the **Tangential momentum accommodation coefficient** $a_\mathrm{v}$. The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 4.

#### *User defined*

For **User defined** select a **Mean free path definition**—**Standard** (the default) or **Alternate (Shapirov)**. Then enter values for the following. Note that the defaults are different based on the Mean free path definition chosen.

- **Thermal slip coefficient** $\sigma_T$. The defaults are 0.97 for **Standard** and 1.1 for **Alternate (Shapirov)**.
- **Viscous slip coefficient** $\sigma_S$. The defaults are 0.89 for **Standard** and 1 for **Alternate (Shapirov)**.
- **Temperature jump coefficient** $\zeta_T$. The defaults are 1.73 for **Standard** and 1.95 for **Alternate (Shapirov)**.

Theoretical and experimental values of these coefficients for various gas surface combinations are available in Ref. 5. Note that it is more convenient to use the **Alternative (Shapirov)** mean free path definition when using this data.

## *Initial Values*

The **Initial Values** node adds initial values for the velocity field, pressure, and temperature. For the transient solver, these values define the state of the problem at the initial time step; for the stationary solver, they serve as a starting point for the nonlinear solver.

### INITIAL VALUES

Enter values or expressions for the initial estimate the solver uses for the **Velocity field** $\mathbf{u}$, **Pressure** $p$, and **Temperature** $T$.

## *Slip Wall*

Use the **Slip Wall** node to specify a wall with slip adjacent to a solid region in which the heat transfer equations are solved. A wall velocity can be specified along with the slip coefficients.

### SLIP WALL

Enter the components for the **Velocity of moving wall** $\mathbf{u}_\mathbf{w}$. Select the **Slip coefficients**: **Maxwell's model** (the default) or **User defined**. These settings are the same as for External Slip Wall.

## *Periodic Condition*

The **Periodic Condition** node applies periodic boundary conditions for the fluid flow and the heat transfer equations, as appropriate.

For more information, see Periodic Boundary Conditions in the *COMSOL Multiphysics Reference Manual*.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

## *Symmetry*

The **Symmetry** node applies symmetry conditions for the fluid flow and/or the heat transfer equations, as appropriate.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

## *Continuity*

The **Continuity** node can be added to pairs. It prescribes that the temperature field is continuous across the pair. Continuity is only suitable for pairs where the boundaries match.

Since it is not usual to use an assembly to represent the fluid flow domains, **Continuity** is only appropriate between two domains in which **Heat Transfer in Solids** applies.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.

# Theory for the Slip Flow Interface

The Slip Flow Interface theory is described in this section:

- Slip Flow Boundary Conditions
- References for the Slip Flow Interface

If you have the Heat Transfer Module, the **Highly Conductive Layer** node (and subnodes) is also available. The feature and the background theory is described in the *Heat Transfer Module User's Guide*.

## Slip Flow Boundary Conditions

Maxwell was the first person to consider the boundary conditions required for the solution of the Boltzmann equation in the case of a slightly rarefied gas (Ref. 1). The boundary conditions he derived can be used as boundary conditions for the Navier Stokes equations in the slip flow regime, although Maxwell considered the particular case of a monatomic hard-sphere gas, so some generalization is required.

Maxwell's boundary condition takes the form:

$$\mathbf{u}_{\mathrm{slip}} = \frac{G}{\mu}(\boldsymbol{\tau}\mathbf{n} - ((\mathbf{n}^T\boldsymbol{\tau}\,\mathbf{n})\mathbf{n})) + \frac{3}{4}\frac{\mu}{\rho T_g}[\nabla\ - \mathbf{n}(\mathbf{n}\cdot\nabla\ )]\left[T_g - \frac{8}{3}G(\mathbf{n}\cdot\nabla T_g)\right] \quad (7\text{-}1)$$

where $\mathbf{u}_{\mathrm{slip}}$ is the slip velocity, $\mathbf{n}$ is the boundary normal, $\tau$ is the viscous stress tensor, $\mu$ is the viscosity of the gas, $\rho$ is its density, and $T_g$ is its temperature. The factor $G$ (which has dimensions of length) is given by:

$$G = \frac{2 - a_v}{a_v}\lambda$$

where $\lambda$ is the mean free path and $a_v$ is the tangential momentum accommodation coefficient (for a model in which the surface reflects some molecules diffusely and some secularly, this is equivalent to the fraction of molecules which are reflected diffusely).

A slightly different definition of the *mean free path* is used here: in terms of Maxwell's original parameter, $l$, the mean free path is $\lambda = 2l/3$. In Maxwell's original paper, he uses a coordinate based notation, the vector notation is available in Ref. 2.

In Equation 7-1 the left-hand term represents the phenomena of viscous slip, whilst the right-hand term produces thermal slip or transpiration. Maxwell was aware that the temperature of the gas was not necessarily equal to that of the wall but formulated the boundary condition using only the gas temperatures. When the wall temperature is included, the following equations are obtained (Ref. 2 and Ref. 3):

$$\mathbf{u}_{\mathrm{slip}} = \sigma_s \frac{\lambda}{\mu}(\boldsymbol{\tau}\mathbf{n} - ((\mathbf{n}^T \boldsymbol{\tau}\, \mathbf{n})\mathbf{n})) + \sigma_T \frac{\mu}{\rho T_g}[\nabla T_w - (\mathbf{n} \cdot \nabla T_w)\mathbf{n}]$$

$$T_w = T_g - \zeta_T \lambda \mathbf{n} \cdot \nabla T_g$$

where $T_w$ is the wall temperature, $\sigma_s$ is the viscous slip coefficient, $\sigma_T$ is the thermal slip coefficient, and $\zeta_T$ is the temperature jump coefficient. Within a generalized Maxwell's model the three coefficients $\sigma_s$, $\sigma_T$, and $\zeta_T$ are given by:

$$\begin{aligned} \sigma_s &= \frac{2 - a_v}{a_v} \\ \sigma_T &= \frac{3}{4} \\ \zeta_T &= \frac{2 - a_v}{a_v} \frac{2\gamma}{\gamma + 1} \frac{\kappa}{\mu C_p} \end{aligned} \tag{7-2}$$

where $\kappa$ is the thermal conductivity of the gas. The mean free path can be computed from the gas properties using the following equation (Ref. 3):

$$\begin{aligned} \lambda &= \frac{2\mu}{\rho \langle c \rangle} \\ \langle c \rangle &= \left(\frac{8RT}{\pi M_n}\right)^{1/2} = \left(\frac{8p}{\pi\rho}\right)^{1/2} \end{aligned} \tag{7-3}$$

consequently:

$$\lambda = \sqrt{\frac{\pi}{2\rho p}}\mu$$

In some cases an alternative definition of the mean free path, $\lambda'$, is used (as, for example, in Ref. 5):

$$\lambda' = \frac{\sqrt{\pi}}{2}\lambda$$

It is possible to use this definition of the mean free path when entering user defined values for the slip coefficients.

Values of the parameters given in Equation 7-2, are available in Ref. 5, although care should be taken with the slip and temperature jump coefficients to adjust for differences between the author's definition of the mean free path and that used in COMSOL Multiphysics.

Also note that the formulation assumes that the ideal gas laws apply. This assumption is implicit in the derivation of the above equations (Ref. 3) and at the level of approximation of the equations is reasonable.

For mixtures of gases in which concentration gradients exist an additional term should be added to the slip on the wall. At present this feature is not implemented in COMSOL.

## *References for the Slip Flow Interface*

1. J.C. Maxwell, "On Stresses in Rarefied Gases Arising from Inequalities of Temperature," *Phil. Trans. R. Soc. Lond.*, vol. 170, pp. 231–256, 1879.

2. D.A. Lockerby, J. M. Reese, D.R. Emerson, and R.W. Barber, "Velocity Boundary Condition at Solid Walls in Rarefied Gas Calculations," *Phys. Rev. E*, vol. 70, 017303, 2004.

3. E.H. Kennard, *Kinetic Theory of Gases*, McGraw-Hill, New York, 1938.

4. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

5. F. Sharipov, “Data on the Velocity Slip and Temperature Jump on a Gas-Solid Interface,” *J. Phys. Chem. Ref. Data*, vol. 40, no. 2, 023101, 2011.

# 8

# Chemical Species Transport Interfaces

The Microfluidics Module has an enhanced version of the Transport of Diluted Species interface that is available with the basic COMSOL Multiphysics® license. In addition, the Transport of Diluted Species in Porous Media interface is available. Both physics interfaces are found under the **Chemical Species Transport** branch ( ⁙ ).

In this chapter:

- The Transport of Diluted Species Interface
- The Transport of Diluted Species in Porous Media Interface
- Theory for the Transport of Diluted Species Interface

# 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 $i$.

Some features are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit http://www.comsol.com/products/specifications/

### 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.

### TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the check boxes available under **Additional transport mechanisms** to control other transport mechanisms.

Note: Not all additional transport mechanisms listed below are available in all products. For details see http://www.comsol.com/products/specifications/.

- By default, the **Convection** check box is selected. Clear the check box to disable convective transport.
- Select the **Migration in electric field** check box to activate the migration transport of ionic species. See further the theory section Adding Transport Through Migration.

#### *Mass Transport in Porous Media*

The **Mass transport in porous media** check box activates functionality specific to species transport in porous media. When selected, the following transport mechanisms are available:

- Select the **Dispersion in porous media** check box to activate the dispersion mechanism in porous media. See further Dispersion in the theory chapter.
- Select the **Volatilization in partially saturated porous media** check box to model volatilization in partially saturated domains. See further Theory for the Transport of Diluted Species Interface.

The following features are also enabled when selecting the **Mass transport in porous media** check box:

- Adsorption
- Partially Saturated Porous Media
- Porous Media Transport Properties

### CONSISTENT STABILIZATION

To display this sections, click the **Show** button ( 👁 ) and select **Stabilization**.

- When the **Crosswind diffusion** check box 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** $g_{\mathrm{lim}}$. It 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** check box 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 **Convective term**—**Non-conservative form** (the default) or **Conservative form**. The conservative formulation should be used for compressible flow. See Convective Term Formulation for more information.

### DISCRETIZATION

To display this section, click the **Show** button ( 👁 ) and select **Discretization**.

The **Compute boundary fluxes** check box is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option is checked, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the check box 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 non-conservative form.

Also the **Apply smoothing to boundary fluxes** check box is available if the previous check box is checked. 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 **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*.
- Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface
- In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 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**
- *Thin-Layer Diffusion*: Application Library path **COMSOL_Multiphysics/Diffusion/thin_layer_diffusion**

## *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 Media Transport Properties 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 Media Transport Properties** and **Partially Saturated Porous Media** 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 Media Transport Properties**, **No Flux** (the default boundary condition), and . 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

- Theory for the Transport of Diluted Species Interface
- 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:
  http://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, 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. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Adsorption
- Concentration
- Flux
- Flux Discontinuity
- InflowInitial Values
- Initial Values
- Line Mass Source
- Mass-Based Concentrations
- No Flux
- Outflow
- Partially Saturated Porous Media
- Periodic Condition
- Point Mass Source
- Porous Media Transport Properties
- Reactions
- Species Source
- Symmetry
- Thin Diffusion Barrier
- Thin Impermeable Barrier
- Transport Properties
- Volatilization

Some features may require certain add-on modules. See details http://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 2-3 for links to common sections and Table 2-4 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.

## *Transport Properties*

The settings in this node are dependent on the check boxes selected under Transport Mechanisms on 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.

When the **Convection** check box is selected, the Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu. Note that this feature is only available in some COMSOL products. See details: http://www.comsol.com/products/specifications/.

### 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

Select an option from the **Material** list. This selection list can only be used if a material has been added in the Materials node and if that material has a diffusion coefficient defined. Else, you need to type in the diffusivity in the **User Defined** edit field.

Enter the **Diffusion coefficient** $D_c$ for each species. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type —**Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** 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: http://www.comsol.com/products/specifications/.

### MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box 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 **Anisotropic** — and type in the value of expression of the mobility $u_{\mathrm{m,c}}$.

Enter the **Charge number** $z_{\mathrm{c}}$ (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: http://www.comsol.com/products/specifications/.

### EXAMPLE MODELS

*Separation Through Dialysis*: Application Library path **Chemical_Reaction_Engineering_Module/Separation_Processes/dialysis**

Web link: http://www.comsol.com/model/separation-through-dialysis-258

*Transport in an Electrokinetic Valve*: Application Library path **Microfluidics_Module/Fluid_Flow/electrokinetic_valve**

Web link: http://www.comsol.com/model/electrokinetic-valve-603

## *Turbulent Mixing*

Note that the Turbulent Mixing node is only available for some product add-ons. See details: http://www.comsol.com/products/specifications/.

This subnode is available from the context menu (right-click the Transport Properties parent node) as well as from the **Physics** toolbar, **Attributes** menu, if **Convection** is selected as a transport mechanism. 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** $\nu_T$ 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).

*Turbulent Mixing of a Trace Species*: Application Library path **CFD_Module/Single-Phase_Tutorials/turbulent_mixing**

Web link: http://www.comsol.com/model/turbulent-mixing-of-a-trace-species-12727

## *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: kg/m$^3$) and mass fractions (dimensionless) for all species.

### MIXTURE PROPERTIES

The default **Solvent density** $\rho_{\mathrm{solvent}}$ 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 $R$ (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 menu. 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 http://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 the volume of a particular phase.

- 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, $\varepsilon_p$. ($\varepsilon_p$ 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 $\theta$. ($\theta$ equals $\varepsilon_p$ for Saturated Porous Media domains).
- For **Gas phase**, the expressions are multiplied by the gas volume fraction $a_v = \varepsilon_p - \theta$. $a_v$ equals 0 for Saturated Porous Media domains.

### FURTHER READING

See the theory chapter on chemical species transport, starting with the section *Mass Balance Equation*.

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- *Fine Chemical Production in a Plate Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/ Reactors_with_Mass_and_Heat_Transfer/plate_reactor**

Web link:
http://www.comsol.com/model/fine-chemical-production-in-a-plate-reactor-8589

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## *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.

## *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** check box 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

This section in the settings is only available for some products. Search for “Inflow” on the page: http://www.comsol.com/products/specifications/ for more details on availability.

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints. The other option, **Flux (Danckwerts)** can be more stable and fast to solve when high reaction rates are anticipated in the vicinity of the inlet. Oscillations on the solutions can also be avoided in such cases. The latter condition uses a flux boundary condition based on the velocity across the boundary and the concentration values. See further details in the theory section.

### 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.

### FURTHER READING

See the theory chapter in the section .

## *Outflow*

This node is not available if **Diffusion** only is included in the model.

Set this condition at outlets where species are transported out of the model domain by fluid motion. It is assumed that convection is the dominating transport mechanism across outflow boundaries, and therefore that diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D\nabla c) = 0$$

## *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 check box 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 check box for the concentration of that species.

### 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.

## *Flux*

This node can be used to specify the total species flux across a boundary. The total flux of species $c$ is defined accordingly:

$$-\mathbf{n} \cdot (c\mathbf{u} - D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi) = N_0$$

where $N_0$ is an arbitrary user-specified flux expression (SI unit: mol/(m$^2$·s)). For example, $N_0$ can represent a flux from or into a much larger surrounding environment, a phase change, or a flux due to chemical reactions. $N_0$ can also be a function of the concentration and the electric potential (if the mass transport includes migration of ionic species).

When diffusion is the only transport mechanism present, the flux condition is extended to include a mass transfer term to describe flux into a surrounding environment:

$$-\mathbf{n}\cdot(-D\nabla c) = N_0 + k_c(c_b - c)$$

where $k_c$ is a mass transfer coefficient (SI unit: m/s), and $c_b$ is the concentration (SI unit: mol/m$^3$) in the surroundings of the modeled system (the bulk concentration). The mass transfer coefficient (to be specified) is often given by boundary-layer theory.

#### INWARD FLUX

This is used to individually specify the flux of each species. To use another boundary condition for a specific species, click to clear the check box for the mass fraction of that species.

Note: Use a minus sign when specifying a flux leaving the system.

### *Symmetry*

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric, that is, where there is no mass flux in the normal direction across the boundary.

This boundary condition is identical to that of the No Flux node, but applies to all species and cannot be applied to individual species.

### *Flux Discontinuity*

This node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n}\cdot(\mathbf{N}_d - \mathbf{N}_u) = N_0 \qquad \mathbf{N} = (c\mathbf{u} - D\nabla c - zu_m Fc\nabla\phi)$$

where the value $N_0$ (SI unit: mol/(m$^2$·s)) specifies the jump in 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 check box 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 check box for the flux discontinuity of that species.

## *Periodic Condition*

The **Periodic Condition** node can be used to define periodicity or antiperiodicity between two boundaries. The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that can each consist of several connected boundaries. For more complex geometries, it might be necessary to add the **Destination Selection** subnode, which is available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

With this subnode, the boundaries that constitute the source and destination surfaces can be manually specified.

### 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*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

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

For the “Reacting Flow in Porous Media, Diluted Species” interface, which is available in some add-on products, the **Line Mass Source** node is available in two versions, 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 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*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

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

For the “Reacting Flow in Porous Media, Diluted Species” interface, which is available in some add-on products, the **Point Mass Source** node is available in two versions, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

### SPECIES SOURCE

Enter the source strength, $\dot{q}_{\mathrm{p,c}}$ , 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*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to set up mass transport across boundaries where both convective inflow and outflow can occur. Use this boundary condition to specify an exterior species concentration 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 provided as a model input to the Transport of Diluted Species interface.

### 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. To set up the node, specify the layer thickness and a diffusion coefficient for each transported species.

### THIN DIFFUSION BARRIER

Enter a **Layer thickness** $d_\mathrm{s}$ (SI unit: m). The default is 0.005 m (5 mm). Enter a **Diffusion coefficient** $D_{\mathrm{s,c}}$ (SI unit: $\mathrm{m^2/s}$). The default is 0.

## *Thin Impermeable Barrier*

This feature models a thin mass transfer barrier. The feature is available on interior boundaries and introduces a discontinuity in the concentration across the boundary. On each side of the boundary, a no-flux condition is prescribed for the mass transport. The Thin Impermeable Barrier boundary 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 or Rotating Interior Wall feature in order to model a thin solid wall.

## *Equilibrium Reaction*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model an equilibrium reaction in a domain. This feature is available with two species or more.

The equilibrium reaction is defined by the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition) and the stoichiometry of the reaction.

The node solves for an additional degree of freedom (the reaction rate) to fulfill the equilibrium condition at all times in all space coordinates.

If the **Apply equilibrium condition on inflow boundaries** check box 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.

### EQUILIBRIUM CONDITION

The list defaults to **Equilibrium constant** or select **User defined**. For either option, the **Apply equilibrium condition on inflow boundaries** check box is selected by default.

For **Equilibrium constant**, enter an **Equilibrium constant** $K_{\mathrm{eq}}$ (dimensionless). The default is 1. Enter a value or expression for the **Unit activity concentration** $C_{\mathrm{a0}}$ (SI unit: $\mathrm{mol/m^3}$). The default is $1{\cdot}10^{-3}$ $\mathrm{mol/m^3}$. **Equilibrium constant** creates an equilibrium condition based on the stoichiometric coefficients, the species activities, and the law of mass action.

For **User defined**, enter an **Equilibrium expression** $E_{\mathrm{eq}}$ (dimensionless).

### STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient $\nu_{\mathrm{c}}$ (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 Equilibrium Reaction*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model an equilibrium reaction on a boundary (surface). The settings for this node are similar to Equilibrium Reaction.

### *Porous Electrode Coupling*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

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 non-negligible total mass source or sink, which is often the case in gas diffusion electrodes, you need to also add a corresponding Porous Electrode Coupling node in the Fluid Flow interface.

### *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** ($i_{\mathrm{loc}}$, SI unit: $\mathrm{A/m^2}$) or **Porous Electrode Reaction** nodes ($i_{\mathrm{v}}$, SI unit: $\mathrm{A/m^3}$) 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*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

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.

In the Transport of Concentrated Species interface, the molar fluxes are multiplied by the species molar masses to obtain the corresponding mass fluxes.

Note that if you are also modeling the momentum transport and expect a non-negligible 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.

## *Porous Media Transport Properties*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model the concentration of diluted species transported through interstices in porous media. A part form convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and reaction.

### 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.

### MATRIX PROPERTIES

Select an option from the **Porous material** list. The default is **Domain material**.

By default the **Porosity,** $\varepsilon_\mathrm{p}$ (dimensionless) is taken **From material**. For **User defined**, enter a different value. The default is 0.3.

When the **Mass transport in porous media** check box is selected in the **Settings** window of the physics interface, a setting for the **Density** $\rho$ of the porous media is available. By default it is set to be taken **From material**.

### 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

Select a **Fluid material** (when available and applicable).

Specify the **Fluid diffusion coefficient** $D_{\mathrm{F,i}}$ (SI unit: $\mathrm{m^2/s}$). Enter a value or expression for each of the species in the corresponding input field. The default is $1 \times 10^{-9}\ \mathrm{m^2/s}$.

Select the **Effective diffusivity model**: **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{\mathrm{F,i}}$ (dimensionless). The default is 1.

### MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box 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 effective 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 **Anisotropic** — and type in the value of expression of the effective mobility $u_{\mathrm{me,c.}}$

Enter the **Charge number** $z_{\mathrm{c}}$ for each species.

### DISPERSION

This section is available when the **Dispersion in porous media** check box is selected on the **Settings** window for the physics interface.

Select the **Specify dispersion for each species individually** check box to specify the dispersion tensor $D_{\mathrm{D}}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$) for each species separately. The default is to use the same dispersion tensor $D_{\mathrm{D}}$ for all species.

Select an option from the **Dispersion tensor** list—**User defined** (the default) or **Dispersivity**. For **User defined**, use it to specify the dispersion components as user-defined constants or expressions. Select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the properties of the dispersion tensor.

Select **Dispersivity** when **Convection** has been added as the transport mechanism. Specify the dispersivities (SI unit: m) to define the dispersion tensor $D_{\mathrm{D}}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$) together with the velocity field $\mathbf{u}$. 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.

## *Adsorption*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model adsorption of the fluid phase species onto the porous media surface. It is available as a subnode to the Porous Media Transport Properties and the Partially Saturated Porous Media nodes.

Select a **Sorption type** — **Langmuir** (the default), **Freundlich**, 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**:

$$c_P = c_{P\max}\frac{K_L c}{1+K_L c} \qquad \frac{\partial c_P}{\partial c} = \frac{K_L c_{P\max}}{(1+K_L c)^2}$$

  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**:

$$c_P = K_F\left(\frac{c}{c_{ref}}\right)^N \qquad \frac{\partial c_P}{\partial c} = N\frac{c_P}{c} \qquad \text{Freundlich}$$

  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 **User defined**:

$$c_P = K_P c \qquad \frac{\partial c_P}{\partial c} = \frac{\partial}{\partial c}(K_P c) \qquad \text{User defined}$$

  Enter an **Adsorption isotherm** $k_{P,c}$ (SI unit: $m^3/kg$).

For more information, see Adsorption in the theory section.

#### FURTHER READING

See the theory chapter in the section Mass Balance Equation for Transport of Diluted Species in Porous Media.

### *Partially Saturated Porous Media*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

Use this node to model the concentration of diluted species transported by a liquid through in partially filled porous media. The interstices of the porous media contains the liquid carrier phase and gas pockets. A part form convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, reaction, and volatilization.

### 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.

### 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 $\theta = s\varepsilon_\mathrm{p}$.

For **Liquid volume fraction**, enter a value for $\theta$ (dimensionless) between 0 and the value of porosity. The saturation is then computed from the porosity and the liquid volume fraction as $s = \theta\varepsilon_\mathrm{p}$.

Select a **Fluid fraction time change**: **Fluid fraction constant in time** (the default), **Time change in fluid fraction**, or **Time change in pressure head**.

- For **Time change in fluid fraction**, enter $\mathrm{d}\theta/\mathrm{d}t$ (SI unit: 1/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** $C_\mathrm{m}$ (SI unit: 1/m).

### 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

Select a **Liquid material** from the list.

Specify the **Liquid diffusion coefficient** $D_{L,c}$ (SI unit: $m^2/s$). Enter a value or expression for each of the species in the corresponding input field. The default is 1 x $10^{-9}$ $m^2/s$.

Select the **Effective diffusivity model, liquid**: **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined**. For **Tortuosity model**, enter a value for $\tau_{L,c}$ (dimensionless). The default is 1.

When the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface, also define the **Gas material**, **Gas diffusion coefficient**, and **Effective diffusivity model, gas**.

### MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. It is similar to that in **Porous Media Transport Properties** feature. Select the source of electric field from the **Electric potential** list. The default selection to **Mobility** is the **Nernst-Einstein relation**.

### DISPERSION

This section is available when the **Dispersion in porous media** check box is selected on the **Settings** window for the physics interface. The settings are the same as for Porous Media Transport Properties.

### VOLATILIZATION

This section is available when the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface.

Enter a value for the **Volatilization** $k_{G,c}$ (dimensionless) for each species.

## *Volatilization*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

This feature is available when the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface.

Use the boundary condition to model a thin layer through which mass is transported by volatilization only. To set up the node, specify the layer thickness and the atmospheric concentration of each species in the thin layer for each transported species.

### VOLATILIZATION

Enter a **Layer thickness** $d_s$ and the atmospheric concentration for each species. The **Gas diffusion coefficient** $D_{G,c}$ (SI unit: $m^2/s$) and the **Volatilization** coefficient $k_{G,c}$ (dimensionless) for each species are taken from the adjacent **Partially Saturated Porous Media** domain.

## *Reactive Pellet Bed*

This feature is only available if you are licensed to use the Chemical Reaction Engineering Module. See details: http://www.comsol.com/products/specifications.

Use this feature to model packed bed reactors with catalytic pellets. For details, see the section Theory for the Reactive Pellet Bed. By default, subnodes for Reactions and  are added.

### BED PARAMETERS

Here you can specify the bed porosity, which is the void fraction in the packed bed structure. Select **From densities** to calculate the porosity from the bed density and the individual pellet density. Select **User defined** to specify the porosity directly.

### PELLET SHAPE AND SIZE

The default shape is spherical. Cylinders, flakes, and user-defined shapes can also be selected. A uniform pellet size or a discrete size distribution can be selected. Select a **Pellet size distribution** — **Uniform size** (the default), **Two sizes**, **Three sizes**, **Four sizes**, or **Five sizes** to select up to five different particle sizes.

Depending on the shape selection, equivalent radii or volumes and surface areas will be required as input. If a size distribution is selected, the volume percentage of each size is required as input.

Note that different chemical reactions can be specified for each pellet size if a distribution is specified.

### SURFACE SPECIES

In order to add surface species, click the **Add** button and enter the species name in the **Surface species** table. Added surface species are be available inside all pellet types defined in the **Pellet Shape and Size** section, but not in the bulk fluid.

For each pellet type, specify the **Reactive specific surface area**, $S_{b,reac}$ (SI unit: 1/m), corresponding to the surface area, per volume, available for surface reactions.

### PELLET PARAMETERS

Enter a **Pellet porosity** $\varepsilon_{\mathrm{pe}}$ (dimensionless) to specify the porosity of the pellet internals.

Select **Diffusion model—Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined** to describe the effective correction of the diffusion coefficient in the pellet. In the case of the **Tortuosity model**, a value for the tortuosity $\tau_{\mathrm{pe}}$ within the pellet is required.

Enter also the **Diffusion coefficient** $D_{\mathrm{pe,c}}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$). If a **User defined** diffusion model is selected, an **Effective diffusion coefficient** $D_{\mathrm{peff,c}}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$) is entered. The default value is $1 \cdot 10^{-9}\ \mathrm{m}^2/\mathrm{s}$ in both cases.

### PELLET-FLUID SURFACE

For the coupling of concentration between the pellet internals and the surrounding fluid, two **Coupling type** options are available:

- **Continuous concentration**, assuming that all resistance to mass transfer to/from the pellet is within the pellet and no resistance to pellet-fluid mass transfer is on the bulk fluid side. The concentration in the fluid will thus be equal to that in the pellet pore just at the pellet surface: $c_{\mathrm{pe},i} = c_i$. This constraint also automatically ensures flux continuity between the internal pellet domain and the free fluid domain through so-called reaction forces in the finite element formulation.
- **Film resistance (mass flux)**: The flux of mass across the pellet-fluid interface into the pellet is possibly rate determined on the bulk fluid side, by film resistance. The resistance is expressed in terms of a film mass transfer coefficient, $h_{D\mathrm{i}}$, such that:

$$N_{i,\mathrm{inward}} = h_{D,i}(c_i - c_{\mathrm{pe},i})\,.$$

The **Film resistance (mass flux)** option computes the inward surface flux, $N_{\mathrm{i,inward}}=h_{\mathrm{Di}}(c_{\mathrm{i}}-c_{\mathrm{pe,i}})$. $h_{\mathrm{Di}}$ is the mass transfer coefficient (SI unit: m/s) and is calculated with the default **Automatic** setting from a dimensionless **Sherwood number expression** or with **User defined** mass transfer coefficients.

The **Active specific surface area** (SI unit: $\mathrm{m}^{-1}$) is required to couple the mass transfer between the pellets and the bed fluid. Select either the **Automatic** setting that calculates the specific surface area from the shape information given above. User defined is also available for explicit surface area specification.

The **Sherwood number expression** can be computed from three available expressions: **Frössling**, **Rosner**, and **Garner and Keey**. The Frössling equation is the default and probably the most commonly used for packed spheres. All of these are based on the dimensionless Reynolds, Re, and Schmidt, Sc, numbers, which are computed from

**Density** and **Dynamic viscosity**. Select these to be taken either **From material** or choose the **User defined** alternative.

### PELLET DISCRETIZATION

The extra dimension in the pellet needs to be discretized into elements. Select a **Distribution** — **Cubic root sequence** (the default), **Linear**, or **Square root sequence**. Enter the **Number of elements** $N_{\text{elem}}$.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. See the details about the different constraint settings in the section Constraint Reaction Terms.

### FURTHER READING

Theory for the Reactive Pellet Bed in the Theory section of this manual.

For an application using the Reactive Pellet Bed feature, see

*A Multiscale 3D Packed Bed Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/packed_bed_reactor_3d**

- Web link: http://www.comsol.com/model/a-multiscale-3d-packed-bed-reactor-17019

## *Reactions*

The Reactions subfeature to the Reactive Pellet Bed is used to define reaction terms to the transport within the reactive pellets. The feature also defines the corresponding averaged heat sources to be applied to heat transport in the bulk fluid.

### DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern source terms 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 $R$ (SI unit: mol/(m$^3$·s)) for species $i$ using a value or an expression. One reaction rate per species and pellet type can be entered.

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 menu. For an example, see the application *Fine Chemical Production in a Plate Reactor* as linked below.

### SURFACE REACTION RATES

The section is available when one or more surface species have been added in the **Surface Species** section of the Reactive Pellet Bed feature.

Specify the rate expression $R$ (SI unit: mol/(m$^2$·s)) corresponding to the surface reaction rate of each volumetric species $i$ participating in the surface reaction. Furthermore, specify the surface reaction rates for the participating surface species in the corresponding table.

If several pellet types have been defined, one set of surface reaction rates per pellet type can be defined.

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 menu.

### HEAT SOURCE

Specify the heat source originating from the heat of reaction of the chemical reactions inside the pellet can be specified. Both heat sources from reactions in the fluid, and heat sources resulting from surface reactions can be defined. When using several pellet types, heat sources for each type can be added.

The heat sources are most conveniently picked up from a Chemistry feature that defines the reaction rate and the heat of reactions. In that case, the Rate expression can be selected from the drop-down menu. Else it can be set to User Defined.

The defined heat source can be used by a Heat Source feature in any of the heat transfer interfaces.

## *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 strain can be written as

$$\varepsilon_{\mathrm{hs}} = \beta_h(c_{\mathrm{mo}} - c_{\mathrm{mo,ref}})$$

where $\beta_{\mathrm{h}}$ is the coefficient of hygroscopic swelling, $c_{\mathrm{mo}}$ is the moisture concentration, and $c_{\mathrm{mo,ref}}$ is the strain-free reference concentration.

It 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 See http://www.comsol.com/products/specifications/.

#### FURTHER READING

More information about how to use hygroscopic swelling can be found in Hygroscopic Swelling Coupling section in the *Structural Mechanics Module User's Guide*.

More information about multiphysics coupling nodes can be found in the section The Multiphysics Node.

### *Fracture*

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

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.

#### FRACTURE PROPERTIES

Specify a value for the **Fracture thickness** $d_{\mathrm{fr}}$.

#### POROUS MATERIAL

Select an option from the **Porous material** list. The default is **Domain material**.

By default the **Porosity,** $\varepsilon_{\mathrm{p}}$ (dimensionless) is taken **From material**. Select **User defined** to enter a different value or expression.

#### CONVECTION

Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use a Fracture Flow 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.

The settings for the **Diffusion**, and **Dispersion** sections are the same as for Porous Media Transport Properties.

# 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 as well as migration due to an electric field. The physics interface assumes that all species present are dilute; that is, that their concentration is small 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 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
- Convective Term Formulation
- Crosswind Diffusion
- Mass Balance Equation
- Mass Sources for Species Transport
- Solving a Diffusion Equation Only
- References

The section also includes the theory for the 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
- 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 $i$:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \tag{8-1}$$

Equation 8-1 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 velocity vector (SI unit: m/s)

The flux vector $\mathbf{N}$ (SI unit: mol/(m$^2$·s)) is associated with the mass balance equation above and used in boundary conditions and flux computations. For the case where the diffusion and convection are the only transport mechanisms, the flux vector is defined as

$$\mathbf{N}_i = -D \nabla c + \mathbf{u} c \tag{8-2}$$

If *Migration in Electric Fields* is activated, the flux vector is amended with the migration term as shown in the section Adding Transport Through Migration.

The first term on the left side of Equation 8-1 corresponds to the accumulation (or indeed consumption) of the species.

The second term accounts for the diffusive transport, accounting for the interaction between the dilute species and the solvent. An input field for the diffusion coefficient is available. Anisotropic diffusion coefficient tensor input is supported.

The third term on the left side of Equation 8-1 describes the convective transport due to a velocity field $\mathbf{u}$. This field can be expressed analytically or obtained from coupling this physics interface to one that computes fluid flow, such as *Laminar Flow*.

On the right-hand side of the mass balance equation (Equation 8-1), $R_i$ 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, which has a field for specifying a reaction equation 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, $\nu_i$ (dimensionless), of the reaction; the species activities of the reacting species $a_i$ (dimensionless); and an equilibrium constant, $K_{eq}$ (1) according to:

$$K_{\mathrm{eq}} = \frac{\prod\limits_{i \in \text{products}} a_i^{\nu_i}}{\prod\limits_{i \in \text{reactants}} a_i^{-\nu_i}}$$

where the species activities are defined as

$$a_i = \gamma_{c,i}\frac{c_i}{c_{\mathrm{a0}}}$$

where $c_{a0}$ (SI unit: $\mathrm{mol/m^3}$) 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:

$$K_{\mathrm{eq}} = \prod_i a_i^{\nu_i}$$

$\gamma_{c,i}$ is set to unity when the Equilibrium constant is selected on 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 non-equilibrium reaction rates set to zero. Manual scaling of the reaction rate dependent variables is needed in this study step.

## *Convective Term Formulation*

The default node attributed to The Transport of Diluted Species Interface assumes chemical species transport through diffusion and convection (a check box to activate migration is available) and implements the mass balance equation in Equation 8-1.

There are two ways to present a mass balance where chemical species transport occurs through diffusion and convection. These are the non-conservative and conservative formulations of the convective term:

$$\text{non-conservative: } \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot (D \nabla c) + R \tag{8-3}$$

$$\text{conservative: } \frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}) = \nabla \cdot (D \nabla c) + R \tag{8-4}$$

and each is treated slightly differently by the solver algorithms. In these equations $D$ (SI unit: $\mathrm{m^2/s}$) is the diffusion coefficient, $R$ (SI unit: $\mathrm{mol/(m^3 \cdot s)}$) is a production or consumption rate expression, and $\mathbf{u}$ (SI unit: m/s) is the solvent velocity field. The diffusion process can be anisotropic, in which case $D$ is a tensor.

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c\nabla\cdot\mathbf{u}$, would equal zero for an incompressible fluid and would result in the non-conservative formulation above. This is in fact the default formulation in this physics interface and ensures that nonphysical source terms do not emerge from a solution for the flow field. 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 8-3 and Equation 8-4 by clearing the Convection check box in the Transport Mechanisms section for The Transport of Diluted Species Interface. The equation then becomes

$$\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) + R$$

## *Mass Sources for Species Transport*

There are two types of mass sources in the Transport of Diluted Species interface: point sources and line sources.

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**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 http://www.comsol.com/products/specifications/

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### POINT SOURCE

A point source is theoretically formed by assuming a mass injection/ejection, $\dot{Q}_{\mathrm{c}}$ (SI unit: mol/(m$^3$·s)), in a small volume $\delta V$ and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_{\mathrm{p,c}}$ (SI unit: mol/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q}_{\mathrm{c}} = \dot{q}_{\mathrm{p,c}} \tag{8-5}$$

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

$$\dot{q}_{\mathrm{p,c}}\mathrm{test}(c)$$

is added at a point in the geometry. As can be seen from Equation 8-5, $\dot{Q}_{\mathrm{c}}$ must tend to plus or minus infinity as $\delta V$ 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 8-5 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 $\dot{Q}_{l,c}$ (SI unit: mol/(m$^3$·s)), located within a tube with cross section $\delta S$ and then letting $\delta S$ 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

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q}_{l,c} = \dot{q}_{l,c} \tag{8-6}$$

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

$$\dot{q}_{l,c}\mathrm{test}(c)$$

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.

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For feature node information, see Line Mass Source and Point Mass Source in the *COMSOL Multiphysics Reference Manual*.

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## *Adding Transport Through Migration*

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**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 http://www.comsol.com/products/specifications/

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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 check box under the Transport Mechanisms section for the physics interface. The mass balance then becomes:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V + c_i \mathbf{u}) = R_i \tag{8-7}$$

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

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.

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**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.

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## *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 electro-active 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:

$$\mathbf{i} = F\sum_j -z_j^2 u_{\mathrm{m},j} F c_j \nabla\phi \tag{8-8}$$

Equation 8-8 is simply Ohm’s law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa\nabla\phi \tag{8-9}$$

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 8-9, yields:

$$\nabla\cdot(-\kappa\nabla\phi) = 0 \tag{8-10}$$

Equation 8-10 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 Péclèt 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 Péclèt 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 under-resolved 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 inlet concentrations and the fluid velocity. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet concentrations to domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an inlet concentration $c_{i,0}$, the Danckwerts inflow boundary condition reads

$$\mathbf{n}\cdot\mathbf{N}_i = \mathbf{n}\cdot(\mathbf{u}\, c_{i,0})$$

## *Mass Balance Equation for Transport of Diluted Species in Porous Media*

#### VARIABLY SATURATED POROUS MEDIA

The following equations for the 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:

$$\begin{aligned}\frac{\partial}{\partial t}(\theta c_i) + \frac{\partial}{\partial t}(\rho_{\mathrm{b}} c_{\mathrm{P},\,i}) + \frac{\partial}{\partial t}(a_{\mathrm{v}} c_{\mathrm{G},\,i}) + \mathbf{u}\cdot\nabla c_i &= \\ \nabla\cdot[(D_{\mathrm{D},\,i} + D_{\mathrm{e},\,i})\nabla c_i] + R_i + S_i&\end{aligned} \tag{8-11}$$

On the left-hand side of Equation 8-11, 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 8-11 $c_i$ denotes the concentration of species $i$ in the liquid (SI unit: $\mathrm{mol/m^3}$), $c_{\mathrm{P},\,i}$ the amount adsorbed to (or desorbed from) solid particles (moles per unit dry weight of the solid), and $c_{\mathrm{G},\,i}$ the concentration of species $i$ in the gas phase.

The equation balances the mass transport throughout the porous medium using the porosity $\varepsilon_\mathrm{p}$, the liquid volume fraction $\theta$; the bulk (or drained) density, $\rho_\mathrm{b} = (1-\varepsilon_\mathrm{p})\rho$, and the solid phase density $\rho$ (SI unit: $\mathrm{kg/m^3}$).

For saturated porous media, the liquid volume fraction $\theta$ is equal to the porosity $\varepsilon_\mathrm{p}$, but for partially saturated porous media, they are related by the saturation $s$ as $\theta = s\varepsilon_\mathrm{p}$. The resulting gas volume fraction is $a_\mathrm{v} = \varepsilon_\mathrm{p} - \theta = (1\text{-}s)\varepsilon_\mathrm{p}$.

On the right-hand side of Equation 8-11, the first term introduces the spreading of species due to mechanical mixing as well as from diffusion and volatilization to the gas phase. The tensor is denoted $D_\mathrm{D}$ (SI unit: $\mathrm{m^2/s}$) and the effective diffusion by $D_\mathrm{e}$ (SI unit: $\mathrm{m^2/s}$).

The last two terms on the right-hand side of Equation 8-11 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 $\mathrm{S}_i$ is an arbitrary source term, for example due to a fluid flow source or sink.

In order to solve for the solute concentration of species $i$, $c_i$, the solute mass sorbed to solids $c_{\mathrm{P},i}$ and dissolved in the gas-phase $c_{\mathrm{G},i}$ are assumed to be functions of $c_i$. Expanding the time-dependent terms gives

$$\begin{aligned}&\frac{\partial}{\partial t}(\theta c_i) + \frac{\partial}{\partial t}(\rho_\mathrm{b} c_{\mathrm{P},\,i}) + \frac{\partial}{\partial t}(a_\mathrm{v} c_{\mathrm{G},\,i}) = \\ &(\theta + \rho_\mathrm{b} k_{P,\,i} + a_\mathrm{v} k_{G,\,i})\frac{\partial c_i}{\partial t} + (1 - k_{\mathrm{G},\,i})c_i\frac{\partial\theta}{\partial t} - (\rho_\mathrm{P} c_{\mathrm{P},\,i} - k_{\mathrm{G},\,i}c_i)\frac{\partial\varepsilon_\mathrm{p}}{\partial t}\end{aligned} \tag{8-12}$$

where $k_{\mathrm{P},i} = \partial c_{\mathrm{P},i}/\partial c_i$ is the adsorption isotherm and $k_{\mathrm{G},i} = \partial c_{\mathrm{G},i}/\partial c_i$ is the linear volatilization. Equation 8-11 can then be written as

$$\begin{aligned}&(\theta + \rho_\mathrm{b} k_{\mathrm{P},\,i} + a_\mathrm{v} k_{\mathrm{G},\,i})\frac{\partial c_i}{\partial t} + (1 - k_{\mathrm{G},\,i})c_i\frac{\partial\theta}{\partial t} - (\rho_\mathrm{P} c_{\mathrm{P},\,i} - k_{\mathrm{G},\,i}c_i)\frac{\partial\varepsilon_\mathrm{p}}{\partial t} + \mathbf{u}\cdot\nabla c_i \\ &= \nabla\cdot[(D_\mathrm{D} + D_\mathrm{e})\nabla c_i] + R_i + S_i\end{aligned} \tag{8-13}$$

### SATURATED POROUS MEDIA

In the case of transport in a saturated porous medium, $\theta = \varepsilon_\mathrm{p}$ and the governing equations are

$$
(\varepsilon_\mathrm{p} + \rho_\mathrm{b} k_{\mathrm{P},\,i}) \frac{\partial c_i}{\partial t} + (c_i - \rho_\mathrm{P} c_{\mathrm{P},\,i}) \frac{\partial \varepsilon_\mathrm{p}}{\partial t} + \mathbf{u} \cdot \nabla c_i = \\
\nabla \cdot [(D_{\mathrm{D},\,i} + \theta \tau_{\mathrm{F},\,i} D_{\mathrm{F},\,i}) \nabla c_i] + R_i + S_i \tag{8-14}
$$

### *Convection in Porous Media*

Convection 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 $\mathbf{u}_\mathrm{a}$, provides an estimate of the fluid velocity within the pores:

$$
\mathbf{u}_\mathrm{a} = \frac{\mathbf{u}}{\varepsilon_\mathrm{p}} \qquad \text{Saturated}
$$

$$
\mathbf{u}_\mathrm{a} = \frac{\mathbf{u}}{\theta} \qquad \text{Partially saturated}
$$

where $\varepsilon_\mathrm{p}$ is the porosity and $\theta = s\varepsilon_\mathrm{p}$ the liquid volume fraction, and $s$ the saturation, a dimensionless number between 0 and 1.

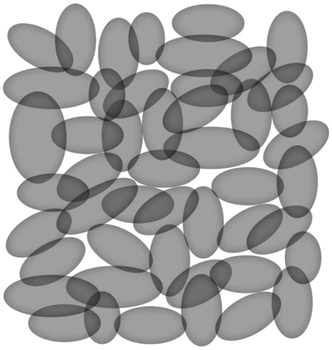

*Figure 8-1: A block of a porous medium consisting of solids and the pore space between the solid grains. The average linear velocity describes how fast the fluid moves within the pores. The Darcy velocity attributes this flow over the entire fluid-solid face.*

### CONVECTIVE TERM FORMULATION

The Transport of Diluted Species in Porous Media interface includes two formulations of the convective term. The conservative formulation of the species equations in Equation 8-11 is written as:

$$\frac{\partial}{\partial t}(\theta c_i) + \frac{\partial}{\partial t}(\rho_b c_{P,i}) + \frac{\partial}{\partial t}(a_v c_{G,i}) + \nabla \cdot \mathbf{u} c_i = \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_i] + R_i + S_i \tag{8-15}$$

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 non-conservative formulation described in Equation 8-11.

When using the non-conservative formulation, which is the default, the fluid is assumed incompressible and divergence free: $\nabla \cdot \mathbf{u} = 0$. The non-conservative 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 **Non-conservative form** (the default) or **Conservative form**. 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. Depending on the transport of diluted species occurs in free flow, saturated or partially saturated porous media, the effective diffusivity is defined as:

$$D_e = D_L \qquad \text{Free Flow}$$

$$D_e = \frac{\varepsilon_p}{\tau_L} D_L \qquad \text{Saturated Porous Media}$$

$$D_e = \frac{\theta}{\tau_L} D_L \qquad \text{Partially Saturated Porous Media}$$

$$D_e = \frac{\theta}{\tau_L} D_L + \frac{a_v}{\tau_G} k_G D_G \qquad \text{Partially Saturated with Volatilization}$$

Here $D_L$ and $D_G$ are the single-phase diffusion coefficients for the species diluted in pure liquid and gas phases respectively (SI unit: $m^2/s$), and $\tau_L$ and $\tau_G$ 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. 12):

$$\tau_F = \theta^{-7/3}\varepsilon^2 \, , \, \tau_G = a_v{}^{-7/3}\varepsilon^2$$

and Bruggeman model

$$\tau_F = \theta^{-5/2}\varepsilon^2 \, , \, \tau_G = a_v{}^{-5/2}\varepsilon^2$$

For saturated porous media $\theta = \varepsilon_p$. The fluid tortuosity for the Millington and Quirk model is

$$\tau_F = \varepsilon_p{}^{-1/3}$$

and for the Bruggeman model the tortuosity is defined as

$$\tau_F = \varepsilon_p{}^{-1/2}$$

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 small.

The spreading of mass, as species 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 is small relative to the mechanical dispersion, except at very low fluid velocities.

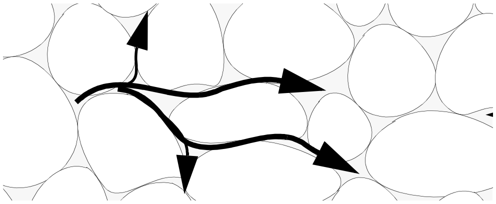

*Figure 8-2: Spreading of fluid around solid particles in a porous medium.*

is controlled through the dispersion tensor $D_{\mathrm{D}}$. 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. 9):

$$D_{\mathrm{D}ii} = \alpha_{\mathrm{L}}\frac{u_i^2}{|\mathbf{u}|} + \alpha_{\mathrm{T}}\frac{u_j^2}{|\mathbf{u}|}$$

$$D_{\mathrm{D}ij} = D_{\mathrm{D}ji} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}})\frac{u_i u_j}{|\mathbf{u}|}$$

In these equations, $D_{\mathrm{D}ii}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$) are the principal components of the dispersivity tensor, and $D_{\mathrm{D}ji}$ and $D_{\mathrm{D}ji}$ are the cross terms. The parameters $\alpha_{\mathrm{L}}$ and $\alpha_{\mathrm{T}}$ (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. 10) can be used. Consider a transverse isotropic media, where the strata are piled up in the z direction, the dispersivity tensor components are:

$$\begin{aligned}
D_{\mathrm{L}xx} &= \alpha_1\frac{u^2}{|\mathbf{u}|} + \alpha_2\frac{v^2}{|\mathbf{u}|} + \alpha_3\frac{w^2}{|\mathbf{u}|} \\
D_{\mathrm{L}yy} &= \alpha_1\frac{v^2}{|\mathbf{u}|} + \alpha_2\frac{u^2}{|\mathbf{u}|} + \alpha_3\frac{w^2}{|\mathbf{u}|} \\
D_{\mathrm{L}zz} &= \alpha_1\frac{w^2}{|\mathbf{u}|} + \alpha_3\frac{u^2}{|\mathbf{u}|} + \alpha_3\frac{v^2}{|\mathbf{u}|} \\
D_{\mathrm{L}xy} &= D_{\mathrm{L}yx} = (\alpha_1 - \alpha_2)\frac{uv}{|\mathbf{u}|} \\
D_{\mathrm{L}xz} &= D_{\mathrm{L}zx} = (\alpha_1 - \alpha_3)\frac{uw}{|\mathbf{u}|} \\
D_{\mathrm{L}yz} &= D_{\mathrm{L}zy} = (\alpha_1 - \alpha_3)\frac{vw}{|\mathbf{u}|}
\end{aligned} \tag{8-16}$$

In Equation 8-16 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 $\alpha_1$ (SI unit: m) is the longitudinal dispersivity. If $z$ is the vertical axis, $\alpha_2$ and $\alpha_3$ 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. 9 and Ref. 11).

## *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. 6). The Adsorption feature includes three predefined relationships to predict the solid concentrations, $c_{\mathrm{P}i}$ from the concentration in the liquid phase, $c_i$:

$$\begin{array}{llll} c_{\mathrm{P}} = K_P c & \dfrac{\partial c_{\mathrm{P}}}{\partial c} = \dfrac{\partial}{\partial c}(K_P c) & \text{User defined} & \\ c_{\mathrm{P}} = K_{\mathrm{F}}\left(\dfrac{c}{c_{\mathrm{ref}}}\right)^N & \dfrac{\partial c_{\mathrm{P}}}{\partial c} = N\dfrac{c_{\mathrm{P}}}{c} & \text{Freundlich} & (8\text{-}17) \\ c_{\mathrm{P}} = c_{\mathrm{Pmax}}\dfrac{K_{\mathrm{L}}c}{1+K_{\mathrm{L}}c} & \dfrac{\partial c_{\mathrm{P}}}{\partial c} = \dfrac{K_{\mathrm{L}}c_{\mathrm{Pmax}}}{(1+K_{\mathrm{L}}c)^2} & \text{Langmuir} & \end{array}$$

The above equations contains the following parameters:

- User defined isotherm $K_{\mathrm{P}}$ (SI unit: $\mathrm{m^3/kg}$).
- Freundlich: Freundlich constant $K_{\mathrm{F}}$ (SI unit:·mol/kg), Freundlich exponent $N_{\mathrm{F}}$ (dimensionless), and reference concentration $c_{\mathrm{ref}}$ (SI unit: $\mathrm{mol/m^3}$).
- Langmuir: Langmuir constant $K_{\mathrm{L}}$ (SI unit: $\mathrm{m^3/mol}$), and adsorption maximum $c_{\mathrm{Pmax}}$ (SI unit: mol/kg).
- These predefined expressions are adsorption isotherms that describe the amount of species sorbed to the solid. Defined at equilibrium, the switch between liquid and solid phases is instantaneous.

Using a Species Source feature, arbitrary expressions can be entered to define, for example, non-equilibrium and temperature-dependent adsorption laws, including those set out by Fetter (Ref. 7) and Bear and Verruijt (Ref. 8).

The retardation factor, RF, describes how adsorption slows the solute velocity, $\mathbf{u}_{\mathrm{c}}$, relative to the average linear velocity of the fluid, $\mathbf{u}_{\mathrm{a}}$, as in

$$\mathrm{RF} = 1 + \frac{\rho_{\mathrm{b}}}{\theta}\frac{\partial c_{\mathrm{P}}}{\partial c} = \frac{\mathbf{u}_{\mathrm{a}}}{\mathbf{u}_{\mathrm{c}}}$$

If the contaminant moves at the average linear velocity of the fluid for $\mathrm{RF} = 1$. For $\mathrm{RF} > 1$, the contaminant velocity is smaller 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 $\theta$. Similarly, solid phase reaction expressions include the bulk density, $\rho_b$, and gas phase reactions include the gas volume fraction, $a_v$.

## References

1. R. Codina, "A discontinuity-capturing crosswind-dissipation for the finite element solution of the convection-diffusion equation", *Computer Methods in Applied Mechanics and Engineering*, vol. 110, pp. 325–342, 1993.

2. P.V. Danckwerts, "Continuous flow systems: Distribution of residence times", *Chem. Eng. Sci.*, vol. 2, no. 1, 1953.

3. J.M. Coulson and J.F. Richardson, *Chemical Engineering, vol. 2*, 4th ed., Pergamon Press, Oxford, U.K., 1991.

4. J.M. Coulson and J.F. Richardson, *Chemical Engineering, vol. 1*, 4th ed., Pergamon Press, Oxford, U.K., 1991.

5. D.E Rosner, *Transport Processes in Chemically Reacting Flow Systems*, ISBN-13: 978-1483130262, Butterworth-Heinemann, 1986

6. D.M. Mackay, D.L. Freyberg, P.V. Roberts, and J.A. Cherry, "A Natural Gradient Experiment on Solute Transport in a Sand Aquifer: 1. Approach and Overview of Plume Movement", *Water Resourc. Res.*, vol. 22, no. 13, pp. 2017–2030, 1986.

7. C.W. Fetter, *Contaminant Hydrogeology*, Prentice Hall, 1999.

8. J. Bear and A. Verruijt, *Modeling Groundwater Flow and Pollution*, D. Reidel Publishing, 1994.

9. J. Bear, *Hydraulics of Groundwater*, McGraw-Hill, 1979.

10. R.D. Burnett and E.O. Frind, "An Alternating Direction Galerkin Technique for Simulation of Groundwater Contaminant Transport in Three Dimensions: 2. Dimensionality Effects", *Water Resour. Res.*, vol. 23, no. 4, pp. 695–705, 1987.

11. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing, 1972.

12. R.J. Millington and J.M. Quirk, "Permeability of Porous Solids", *Trans. Faraday Soc.*, vol. 57, pp. 1200–1207, 1961.

13. I. Langmuir, “Chemical Reactions at Low Temperatures”, *J. Amer. Chem. Soc.*, vol. 37, 1915.

14. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, Inc., 2007.

# 9

# Glossary

This Glossary of Terms contains finite element modeling terms specific to the Microfluidics Module and its applications. For mathematical terms as well as geometry and CAD terms specific to the COMSOL Multiphysics$^{®}$ software and its documentation, see the glossary in the *COMSOL Multiphysics Reference Manual*. To find references in the documentation set where you can find more information about a given term, see the index.

# Glossary of Terms

**absorption (gas)** Uptake of a gas into the bulk of a liquid. Gas absorption takes place, for example, in the liquid of a scrubber tower where an up-streaming gas is washed by a down-going flow of a scrubber solution.

**adsorption (molecule)** Attachment of a molecule or atom to a solid surface. Adsorption involves a chemical bond between the adsorbed species and the surface.

**ALE** See *arbitrary Lagrangian-Eulerian method.*

**arbitrary Lagrangian-Eulerian (ALE) method** A technique to formulate equations in a mixed kinematical description. An ALE referential coordinate system is typically a mix between the material (Lagrangian) and spatial (Eulerian) coordinate systems.

**biosensor** A general term for sensor devices that either detect biological substances or use antibodies, enzymes, or other biological molecules in their operation. Biosensors are a subcategory of chemical sensors.

**Bond number** A dimensionless number given by the ratio of surface tension forces to body forces (usually gravity) for a two-phase flow. It is also known as the Eötvös number, $\mathrm{Eo}$. At high Bond numbers surface tension has a minimal effect on the flow; at low Bond numbers, surface tension dominates. The Bond number, $\mathrm{Bo}$, is given by:

$$\mathrm{Bo} = \frac{\rho g L^2}{\sigma}$$

where $\rho$ is the density, $g$ is the body force acceleration, $L$ is the characteristic length, and $\sigma$ is the surface tension coefficient. The density can refer to a density difference when considering buoyancy.

**Brinkman equations** A set of equations extending Darcy's law in order to include the transport of momentum through shear in porous media flow.

**capillary number** A dimensionless number given by the ratio of viscous forces to surface tension for a two phase flow. At low capillary numbers flow in porous media is dominated by surface tension. The capillary number, $\mathrm{Ca}$, is given by:

$$\mathrm{Ca} = \frac{\mu v}{\sigma}$$

where $\mu$ is the viscosity, $v$ is the characteristic velocity of the problem, and $\sigma$ is the surface tension coefficient.

**continuum flow** Fluid flow which is well described by approximating the liquid as a continuum with the Navier-Stokes equations.

**convection** Transport of molecules or heat due to the movement of the surrounding medium.

**creeping flow** Models the Navier-Stokes equations without the contribution of the inertia term. This is often referred to as *Stokes flow* and is appropriate for use when viscous flow is dominant, such as in very small channels or microfluidic applications.

**crosswind diffusion** A numerical technique for stabilization of the numeric solution to a convection-dominated PDE by artificially adding diffusion perpendicular to the direction of the streamlines.

**Darcy's Law** Equation that gives the velocity vector as proportional to the pressure gradient. Often used to describe flow in porous media.

**Debye layer** See *electric double layer.*

**dielectrophoresis (DEP)** Migration of polarizable particles in an electrolyte in a nonuniform applied electric field.

**diffusion** Transport of material resulting from the random motion of molecules in the presence of a concentration gradient.

**Dukhin number** A dimensionless number given by the ratio of the surface conductivity contribution to the fluid bulk electrical conductivity contribution in electrokinetic phenomena. The Dukhin number, $\mathrm{Du}$, is given by:

$$\mathrm{Du} = \frac{K^{\sigma}}{K^{B}}$$

where $K^{\sigma}$ is the surface conductivity and $K^{B}$ is the bulk conductivity. For low Dukhin numbers, surface conductivities can be neglected when modeling electrokinetic flows.

**electric double layer (EDL)** Sometimes referred to as the Debye layer. At the contact of a solid and a polar fluid (such as water), the solid acquires an electric charge. This charge attracts ions within the fluid, and a narrow fluid layer of opposite charge, the Stern layer, forms on the boundary. In addition, adjacent to the Stern layer, a wider layer with the same charge as in the Stern layer forms in the fluid. Together, the Stern layer and the wider layer (called the diffuse or Gouy-Chapman layer) form the electric double layer. Due to the close distance between the charges, the Stern layer is fixed on the surface, but the more distant diffuse layer can move.

**electrohydrodynamics** A general term describing phenomena that involve the interaction between solid surfaces, ionic solutions, and applied electric and magnetic fields. It is frequently used in microfluidic devices to manipulate fluids and move particles for sample handling and chemical separation.

**electrokinetics** Study of the motion of charged particles under an applied electric field in moving substances such as water.

**electrokinetic flow** Transport of fluid or charged particles within a fluid by means of electric fields. See also *electroosmosis, electrophoresis, electrothermal flow*, and *dielectrophoresis.*

**electrolyte** A solution that can carry an electric current through the motion of ions.

**electroosmosis** Fluid flow in a narrow channel produced by the movement of the *electric double layer* (EDL) along the channel boundary under the influence of an applied electric field. Also, fluid flow through a membrane under the influence of an applied electric field. See also *electric double layer.*

**electroosmotic flow** See *electroosmosis.*

**electrophoresis** Migration of charged electrolyte ions or particles in an applied electric field.

**electrothermal effects** These effects occur in a conductive fluid where the temperature is modified by Joule heating from an AC electric field. This creates variations in conductivity and permittivity and thus Coulomb and dielectric body forces.

**electrothermal flow** Fluid flow resulting from an applied nonuniform AC electric field on a fluid. The Joule heating changes the fluid's electrical properties locally, and that effect, together with the power gradient of the AC electric field, results in fluid motion.

**electrowetting** The *electrowetting effect* describes the change in solid-electrolyte contact angle that occurs when a potential difference is applied between the solid and the electrolyte.

**electrowetting-on-dielectric (EWOD)** A form of *electrowetting* in which a thin insulating layer separates the conducting solid surface from the electrolyte.

**Eötvös number** See *Bond number.*

**Eulerian frame** A frame of reference with its coordinate axes fixed in space.

**Fick's laws** The first law relates the concentration gradients to the diffusive flux of low concentration solute diluted in a solvent. The second law introduces the first law into a differential material balance for the solute.

**fluid-structure interaction (FSI)** When a flow affects the deformation of a solid object and vice versa.

**free molecular flow** The flow of gas molecules through a geometry which is much smaller than the mean free path (Knudsen number, $Kn>10$). In the free molecular flow regime the gas molecules collide with the walls of the geometry much more frequently than they collide with themselves.

**fully developed laminar flow** Laminar flow along a channel or pipe that has velocity components only in the main direction of the flow. The velocity profile perpendicular to the flow does not change downstream in the flow.

**Gouy-Chapman layer** See *electric double layer (EDL).*

**Hagen-Poiseuille equation** See *Poiseuille's law.*

**Helmholtz-Smoluchowski equation** Gives the velocity of a parallel electroosmotic flow for an applied electric field.

**intrinsic volume averages** The physical properties of the fluid, such as density, viscosity, and pressure.

**Knudsen number** A dimensionless number that provides a measure of how rarefied a gas flow is, in other words, the mean free path of the gas molecules compared to the length scale of the flow. The following equation defines the Knudsen number Kn where $\lambda$ is the mean free path of the molecules and $L$ is a length scale characteristic to the flow.

$$Kn = \frac{\lambda}{L}$$

**Knudsen layer** A layer of rarefied fluid flow that occurs within a few mean free paths of the walls in a gas flow. The continuum Navier-Stokes equations break down in this layer.

**Lagrangian frame** A frame of reference with its coordinate axes fixed in a reference configuration of a deforming material. As the material deforms, the Lagrangian frame deforms with it.

**Laplace number** The Laplace number, La, (also known as the Surataman number, Su) relates the inertial and surface tension forces to the viscous forces. It is used to describe the breakup of liquid jets and sheets: at high Laplace and low Reynolds numbers the Rayleigh Instability occurs, at low Laplace and high Reynolds numbers atomization occurs. The Laplace number is given by:

$$La = \frac{\rho\sigma L}{\mu^2}$$

where $\rho$ is the fluid density, $\sigma$ is the surface tension coefficient, $L$ is the characteristic length scale of the problem, and $\mu$ is the viscosity. The Laplace number is directly related to the Ohnesorge number, Oh, through the equation $\mathrm{La}=1/\mathrm{Oh}^2$.

**Mach number** Ratio of the convective speed, $v$, to the speed of sound in the medium, $a$. The Mach number, $Ma$, is defined by the equation:

$$Ma = \frac{v}{a}$$

**magnetohydrodynamics** Fluid flow phenomena involving magnetic fields.

**magnetophoresis** Migration of magnetic or paramagnetic particles suspended in a fluid as a result of an applied magnetic field. The field must be non-uniform in the case of paramagnetic particles.

**Marangoni effect** Fluid flow parallel to an interface induced by surface tension gradients.

**Marangoni number** Ratio of thermal surface tension forces to viscous forces. The Marangoni number, Mg, is given by:

$$Mg = \frac{d\sigma}{dT}\frac{L\Delta T}{\mu\alpha}$$

where $\sigma$ is the surface tension coefficient, $T$ is the absolute temperature ($\Delta T$ is the characteristic temperature difference), $L$ is the characteristic length, and $\alpha$ is the thermal diffusivity ($\alpha=\kappa/(\rho c_p)$), where $c_p$ is the heat capacity at constant pressure, $\kappa$ is the thermal conductivity, and $\rho$ is the density of the fluid.

**microfluidics** Study of the behavior of fluids at the microscale. Also refers to MEMS fluidic devices.

**migration** The transport of charged species in an electrolyte due to the electric force imposed by the electric field.

**mobility** The relation between the drift velocity of a molecule within a fluid and the applied electric field.

**Newtonian flow** Flow characterized by a constant viscosity or a viscosity that is independent of the shear rate in the fluid.

**Nernst-Plank equation** Flow equation that describes the flux of an ion through diffusion, convection, and migration in an electric field. The equation is valid for diluted electrolytes.

**Ohnesorge number** A dimensionless number relating the inertial and surface tension forces to the viscous forces. Used to describe the breakup of liquid jets and sheets: at low Ohnesorge and Reynolds numbers the Rayleigh instability occurs; at high Ohnesorge and Reynolds numbers atomization occurs. The Ohnesorge number, Oh, is given by:

$$\mathrm{Oh} = \frac{\mu}{\sqrt{\rho\sigma L}}$$

where $\rho$ is the fluid density, $\sigma$ is the surface tension coefficient, $L$ is the characteristic length scale of the problem, and $\mu$ is the viscosity. The Ohnesorge number is directly related to the Laplace number, La, through the equation $\mathrm{Oh}=1/\mathrm{La}^{1/2}$.

**Peclet number** A dimensionless number describing the ratio of convection to diffusion in a fluid flow. The Peclet number, Pe, can be used to describe concentration diffusion or heat diffusion. It is given by:

$$\mathrm{Pe} = \frac{vL}{D}$$

where $v$ is the convective velocity, $L$ is the flow length scale, and $D$ is the diffusion constant.

**Poiseuille's law** Equation that relates the mass rate of flow in a tube as 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.

**Reynolds number** A dimensionless number classifying how laminar or turbulent a flow is. The *Reynolds number* Re is a measure of the relative magnitude of the flow's viscous and inertial forces. It is defined by the following equation where $\rho$ is the fluid density, $\mu$ is the dynamic viscosity, $\nu$ is its kinematic viscosity, $v$ is a velocity characteristic to the flow, and $L$ is a length scale characteristic to the flow.

$$\mathrm{Re} = \frac{\rho v L}{\mu} = \frac{vL}{\nu}$$

**slip flow** Fluid flow that occurs when the *Knudsen number*, Kn, is in the range $0.01<\mathrm{Kn}<0.1$. As a result of rarefaction effects in the *Knudsen layer* the no slip boundary condition fails. The flow outside the Knudsen layer can be represented by the continuum Navier-Stokes equations provided that an appropriate slip boundary condition is used for the fluid flow and the correct temperature jump boundary condition is applied at the interface.

**streamline diffusion** A numerical technique for stabilization of the numeric solution to a convection-dominated PDE by artificially adding diffusion in the direction of the streamlines.

**Stern layer** A layer of immobile ions and associated solvent molecules present at the solid-liquid interface in an electric double layer (EDL).

**Stokes flow** See *creeping flow.*

**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.

**surface tension** Surface tension is a property of the surface of a liquid that allows it to resist an external force. Equivalently it can be through of as the energy per unit area of the liquid surface. It is caused by asymmetries in the cohesive forces between molecules at the surface of the liquid.

**Surataman number** See *Laplace number.*

**transitional flow** Fluid flow that occurs when the *Knudsen number*, Kn, is in the range $0.1<\mathrm{Kn}<10$. In this regime the flow is so rarefied that continuum equations break down completely. However collisions between the molecules are still important, so free molecular flow is not applicable.

**Weber number** A dimensionless number describing the ratio of inertial forces to surface tension forces. The Weber number is given by:

$$\mathrm{We} = \frac{\rho v^2 L}{\sigma}$$

where $\rho$ is the density of the fluid, $v$ is the characteristic velocity of the flow, $L$ is the characteristic length scale, and $\sigma$ is the surface tension coefficient.

**zeta potential** The potential of at the interface between the electric double layer and a solid surface in an electrolyte.

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