

Subsurface Flow Module

User's Guide



Subsurface Flow Module User's Guide

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Introduction

This guide describes the Subsurface Flow Module, an optional add-on package that extends the COMSOL Multiphysics[®] modeling environment with customized physics interfaces for modeling fluid flow below the ground level or in porous media in general. It allows to combine this flow with other phenomena, such as poroelasticity, heat transfer, chemistry, and electromagnetic fields.

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.

- About the Subsurface Flow Module
- Overview of the User's Guide

About the Subsurface Flow Module

In this section:

- How the Subsurface Flow Module Helps Improve Your Modeling
- The Subsurface Flow Module Physics Interface Guide
- Common Physics Interface and Feature Settings and Nodes
- Subsurface Flow Module Study Availability
- The Liquids and Gases Materials Database
- Where Do I Access the Documentation and Application Libraries?



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

How the Subsurface Flow Module Helps Improve Your Modeling

The earth and surrounding planets are a giant laboratory filled with an unlimited array of basic physics and multiphysics interactions. Whether in concert or alone, these physical phenomena alter our access to important resources, affect the quality of the environment, shape the ground beneath our feet on earth, and form other planets.

The Subsurface Flow Module is used in the quantitative investigation of geophysical and environmental phenomena, especially within the area of subsurface flow. The module combines physics interfaces for fundamental processes and links to COMSOL Multiphysics and the other modules for structural mechanics and electromagnetics analyses. New physics represented include heating from radiogenic decay that produces the geotherm, which is the increase in background temperature with depth. You can use the variably saturated flow interfaces to analyze unsaturated zone processes (important to environmental engineers) and two-phase flow (of particular interest in the petroleum industry as well as steam-liquid systems). Important in subsurface flow, the heat transfer and chemical transport interfaces explicitly account for physics in the liquid, solid, and gas phases.

The physics interfaces, options, and functions are tailored to account for subsurface flow and geologic process terminology. The Heat Transfer interfaces, for example, include features to superpose a background geotherm without incorporating it as a

boundary condition. These physics interfaces also include options to automate the calculation of effective thermal properties for multicomponent systems.

The Fluid Flow branch represent a wide range of possibilities. The Richards' Equation interface describes nonlinear flow in variably saturated porous media. The options for saturated porous media include the Darcy's Law interface for slow flow and the Brinkman Equations interface where shear is nonnegligible. The Laminar Flow interface uses the Navier-Stokes equations to cover free flows and the Fracture Flow interface is used for modeling flow in fractures.

The module also treats the transport of chemicals and their reactions with the Chemical Species Transport branch. The Transport of Diluted Species in Porous Media interface account for chemical transfer in solid, liquid, and gas phases for free, saturated, and variably saturated fluid flows. The Subsurface Flow Module Applications Libraries has a number examples linking these physics interfaces together.

The Subsurface Flow Module Physics Interface Guide

The table below lists all the physics interfaces specifically available with this module in addition to the core physics interfaces included in COMSOL Multiphysics. The Subsurface Flow Module enhances the COMSOL Multiphysics basic interfaces regarding the "Transport of Diluted Species" interface and adds the Poroelasticity interface to structural mechanics.

The Subsurface Flow Module has a set of physics interfaces adopted for a broad category of simulations important in earth investigations. These physics interface and models can serve equally well as tools for research, applied investigations, and classroom education.

The predefined physics interfaces available in this module cover three main application areas. The Subsurface Flow Module interfaces are available in 2D, 2D axisymmetry, and 3D. The physics interfaces for heat transfer and species transport are also available in 1D and 1D axisymmetry. All physics interfaces are available for both stationary and time-dependent analyses. The physics interfaces can be combined to model, for

example, reacting systems and nonisothermal flow. Alternatively, predefined multiphysics interfaces can be used.

In the COMSOL Multiphysics Reference Manual:



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

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE							
Chemical Species Transport											
Transport of Diluted Species	:="	tds	all dimensions	stationary; time dependent							
Transport of Diluted Species in Porous Media		tds	all dimensions	stationary; time dependent							
Transport of Diluted Species in Fractures	3	dsf	3D, 2D, 2D axisymmetric	stationary; time dependent							
Reacting Flow	•										
Laminar Flow, Diluted Species ^I			3D, 2D, 2D axisymmetric	stationary; time dependent							
Reacting Flow in	Porous	Media									
Transport of Diluted Species	•	rfds	3D, 2D, 2D axisymmetric	stationary; time dependent							
Fluid Flow	•										
Single-Phase Flow											
Creeping Flow	==	spf	3D, 2D, 2D axisymmetric	stationary; time dependent							

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE		
Laminar Flow ^I	<i>\\\\</i>	spf	3D, 2D, 2D axisymmetric	stationary; time dependent		
Multiphase Flow						
🥦 Phase Transport						
Phase Transport	*	phtr	3D, 2D, 2D axisymmetric	stationary; time dependent		
Phase Transport in Porous Media		phtr	3D, 2D, 2D axisymmetric	stationary; time dependent		
Porous Media and	Subsu	urface Flo	ow			
Brinkman Equations	Ō	br	3D, 2D, 2D axisymmetric	stationary; time dependent		
Darcy's Law	\$	dl	all dimensions	stationary; time dependent		
Fracture Flow	K	esff	3D, 2D, 2D axisymmetric	stationary; time dependent		
Richards' Equation	6	dl	all dimensions	stationary; time dependent		
Multiphase Flow in Porous Media		_	3D, 2D, 2D axisymmetric	stationary; time dependent		
Two-Phase Darcy's Law	\$	tpdl	3D, 2D, 2D axisymmetric	stationary; time dependent		
Free and Porous Media Flow		fp	3D, 2D, 2D axisymmetric	stationary; time dependent		
Nonisothermal Fl	ow					
Brinkman Equations	©		3D, 2D, 2D axissymmetri c	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF		

PHYSICS INTERFACE	ICON	TAG	SPACE	AVAILABLE STUDY TYPE		
THISICS INTERIACE	lcon	140	DIMENSION	AVAILABLE STODT TITE		
Fluid-Structure Interaction						
Shallow Water Equations						
Shallow Water Equations, Time Explicit		swe	ID and 2D	time dependent		
/// Heat Transfer						
Heat Transfer in Solids	(ht	all dimensions	stationary; time dependent		
Heat Transfer in Fluids ^I	∫ ≋	ht	all dimensions	stationary; time dependent		
Heat Transfer in Solids and Fluids ^I	∫ ≊	ht	all dimensions	stationary; time dependent		
Heat Transfer in Fractures) 🚱	htlsh	3D, 2D, 2D axisymmetric	stationary; time dependent; thermal perturbation, frequency domain		
Heat Transfer in Porous Media	/	ht	all dimensions	stationary; time dependent		
Structural Mechanics						
Poroelasticity, Solid	﴿	poro	3D, 2D, 2D axisymmetric	stationary; time dependent		
Poroelasticity, Large Deformation, Solid	\$	poro	3D, 2D, 2D axisymmetric	stationary; time dependent		
This physics interface is included with the core COMSOL package but has added functionality for this module.						

Common Physics Interface and Feature Settings and Nodes

There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in the same way no matter the physics interface or feature being used. There are also some physics feature nodes that display in COMSOL Multiphysics.

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



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

Subsurface Flow Module Study Availability

All the physics interfaces included with the module have the Stationary and Time Dependent preset studies available. Custom studies are also available based on the physics interface.



Studies and Solvers and The Physics Interfaces in the COMSOL Multiphysics Reference Manual

The Liquids and Gases Materials Database

The Liquids and Gases material database provides temperature-dependent fluid dynamic and thermal properties such as dynamic viscosity, heat capacity at constant pressure, density, and thermal conductivity.



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

Where Do I Access the Documentation and Application Libraries?

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



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

THE DOCUMENTATION AND ONLINE HELP

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

Opening Topic-Based Help

The Help window is useful as it is connected to the features in the COMSOL Desktop. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then displays information about that feature (or click a node in the Model Builder followed by the **Help** button (?). This is called *topic-based* (or *context*) help.

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 (2) button.

To open the **Help** window:



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

Opening the Documentation Window

To open the **Documentation** window:

Win

• Press Ctrl+F1.

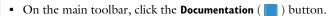
• From the File menu, select Help>Documentation (

Mac

Linux

To open the **Documentation** window:

• Press Ctrl+F1.



• From the main menu, select Help>Documentation.

THE APPLICATION LIBRARIES WINDOW

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

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



The Application Libraries Window in the COMSOL Multiphysics Reference Manual.

Opening the Application Libraries Window

To open the Application Libraries window ():

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

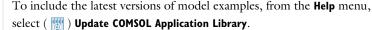
To include the latest versions of model examples, from the File>Help menu, select () Update COMSOL Application Library.



Linux

Win

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



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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 will be sent to you by email. You can also access technical support, software updates, license information, and other resources by registering for a COMSOL Access account.

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Product Updates	www.comsol.com/support/updates	
COMSOL Blog	www.comsol.com/blogs	
Discussion Forum	www.comsol.com/community	
Events	www.comsol.com/events	
COMSOL Application Gallery	www.comsol.com/models	
COMSOL Video Gallery	www.comsol.com/video	
Support Knowledge Base	www.comsol.com/support/knowledgebase	

Overview of the User's Guide

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



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

TABLE OF CONTENTS AND INDEX

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

THE SINGLE-PHASE FLOW BRANCH

The single-phase flow interfaces Laminar Flow and Creeping Flow are described in Chapter Single- and Multiphase Flow Interfaces.

THE MULTIPHASE FLOW BRANCH

The Phase Transport Interfaces section describes the transport of multiple immiscible phases in free and porous media flow.

THE POROUS MEDIA FLOW BRANCH

Porous Media and Subsurface Flow Interfaces chapter describes the following physics interfaces and includes the underlying theory for each physics interface at the end of the chapter.

- The Porous Media and Subsurface Flow group of interfaces estimates the pressure and velocity of fluids flowing in free systems and within the interstices of a porous medium. Theory for the Darcy's Law Interface helps you choose the right physics interface to use.
- The Darcy's Law Interface is for flow in porous media that is relatively slow.
- The Two-Phase Darcy's Law Interface to simulate two-phase slow flow through interstices in a porous medium.
- The Richards' Equation Interface is for variably saturated systems.

- The Fracture Flow Interface is a special application of Darcy's law for modeling flow in fractures.
- The Brinkman Equations Interface is for fast flow in porous media flow.
- The Free and Porous Media Flow Interface is for modeling fluid flow in systems with both free and porous media flow.

THE SHALLOW WATER EQUATIONS BRANCH

The Shallow Water Equations Interface chapter describes the The Shallow Water Equations, Time Explicit Interface and includes the underlying theory. It is suitable in cases where the horizontal length scale is much greater than the vertical length scale.

THE CHEMICAL SPECIES TRANSPORT BRANCH

Chemical Species Transport Interfaces chapter describes the physics interfaces found under the Chemical Species Transport branch when adding a physics interface. The Transport of Diluted Species interface is used to compute 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 computed.

The Transport of Diluted Species in Porous Media Interface characterizes the fate and transport of individual or multiple and interacting chemical species for systems containing fluids, solids, and gases. Theory for the physics interfaces is included at the end of the chapter.

The Transport of Diluted Species in Fractures Interface is used to model the transport of a solute species along thin fractures. The interface takes into account diffusion, dispersion, convection, and chemical reactions in fractures. The fractures are defined by boundaries in 2D and 3D, and the solute species is assumed to be diluted in a solvent. The mass transport equation solved along the fractures is the tangential differential form of the convection-diffusion-reaction equation.

THE HEAT TRANSFER BRANCH

Heat Transfer Interfaces chapter describe the group of interfaces that estimate the temperature distribution in solids, fluids, and fluid-solid systems. The Mechanisms for Heat Transfer helps you choose the physics interface to use. It includes physics interfaces to estimate effective properties in multicomponent systems. All heat transfer interfaces come with interfaces to account for a geotherm brought about through radiogenic decay.

The Heat Transfer Interface models heat transfer by conduction and convection. Surface-to-ambient radiation effects around edges and boundaries can also be

included. The physics interfaces are available in 1D, 2D, and 3D and for axisymmetric models with cylindrical coordinates in 1D and 2D.

The Heat Transfer in Porous Media Interface lets you describe heat transferred both with and without flowing fluids. You can define the velocity in the convective term with any of the flow equations just mentioned or set it with an arbitrary expression. With convective heat transfer, the effective thermal properties also include an option to estimate the dispersion or spreading of heat from small-scale velocity variations.



When you have the Subsurface Flow Module plus the Chemical Reaction Engineering and/or Heat Transfer Modules, the Heat Transfer interface also has extended features available.

THE MULTIPHYSICS COUPLING NODES

In the Multiphysics Interfaces and Couplings chapter the predefined multiphysics interfaces are introduced.

The Poroelasticity Interfaces chapter describes the physics interface for Biot's poroelasticity, and combines Darcy's law with solid mechanics to provide suitable settings to describe the interaction between porous media and fluids.

The Multiphase Flow in Porous Media Interface combines the functionality of the Darcy's Law and Phase Transport in Porous Media interfaces.

The Reacting Flow in Porous Media Interface combines the Brinkman Equations and the Transport of Diluted Species in Porous Media interfaces.

The Nonisothermal Flow, Brinkman Equations Interface couples porous media flow and heat transfer by combining the Brinkman Equations and the Heat Transfer in Porous Media interfaces.

Subsurface Flow Modeling

A variety of modeling techniques are discussed in the following sections:

- Where Do I Start with Subsurface Flow Modeling?
- Selecting the Right Fluid Flow Interface
- Note About the Groundwater Flow Equation
- Pressure, Pressure Head, and Hydraulic Head Formulation
- Gravity Effects

Where Do I Start with Subsurface Flow Modeling?

Before beginning with modeling, it is important to be aware of the following questions:

- Which goal do I pursue with the simulation?
- What accuracy is required from the results?
- Which physical effects play a role?

The first question refers to the results that the simulation should deliver. The system under consideration is often very complex in structure and the physical processes involved. Not everything is relevant for the specific task. Together with the second and third question, the simulation model can then be reduced to the most essential.

Often a 2D or 2D axial symmetric model, sometimes even a 1D model is sufficient. Especially in subsurface flow problems, one has to deal with very large areas. The question is to what extent small-scaled structures are relevant for the result and therefore have to be represented in the geometry. The physical effects to be considered also depend on how accurate the results should be: Does gravity play a role or do I have to take temperature fluctuations into account? These questions should be answered before starting the simulation.

The accuracy of the results also depends on the accuracy of the input quantities. Especially in geophysical questions the exact structure, the material and its properties are not exactly known. Therefore the result cannot be more exact than the accuracy of these and it is not necessary to represent every smallest detail in the model.

Regardless of the above answers, it is always advisable to make the models successively more complex. Complex 3D models are always significantly more computationally demanding and often make high demands on the meshing, whereas in 2D models the focus can be placed on the physical processes and effects. This implies using a simplified model as a starting point in the project. Complexities can then be introduced gradually so that the effect of each refinement of the model description is well understood before introducing new complexities.

Selecting the Right Fluid Flow Interface

The Fluid Flow physics features included with the Subsurface Flow Module are used to characterize movements of liquids, gases, and other flowing media, such as molten rock. The physics interfaces are set up using terms like pressure and hydraulic heads, that are familiar to hydrologists.

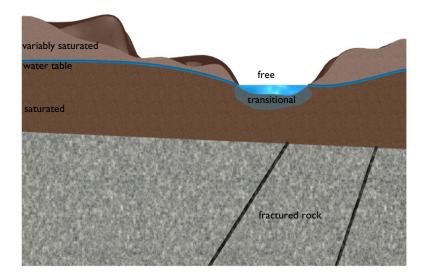


Figure 2-1: Different areas of subsurface flow regimes.

Saturated porous media flow can be modeled through either Darcy's Law or Brinkman's extension to Darcy's Law, depending on the size of the pores involved. If the pore is such that viscous effects to the fluid flow can be ignored, then Darcy's Law can be used, and flow is described exclusively by the pressure variable. If the size of the pores is such that the fluid can impose momentum changes through shear effects, then the Brinkman equations are suitable. They solve for the same variables as the NavierStokes equations, but include terms that consider the porosity of the media the fluid is flowing through.



Read more About Darcian and Non-Darcian Flow and Permeability Models in the Porous Media Flow User's Guide.

In variably saturated porous media flow (usually above the water table), hydraulic properties may change as fluids move through the medium, filling some pores and draining others. Richards' equation is employed to model this type of flow, and the van Genuchten and Brooks and Corey formulations can be applied to take retention in the pores into account. Density, dynamic viscosity, saturated and residual liquid fraction, hydraulic conductivities, and storage models can be provided.

The Fracture Flow interface solves for pressure on internal (2D) boundaries within a 3D matrix and is automatically coupled to the physics describing the porous media flow in the surrounding matrix. This approximation saves you from meshing the actual fractures and the computational resources this entails. If a fluid happens to flow from one medium to the other (and back) in the same model, all of the porous media physics are automatically coupled to descriptions of free flow within the Subsurface Flow Module.

The Navier-Stokes equation describes free flow of liquid. In the above picture it is valid to model the flow in the river bank but it can also be used to model flow through the porous medium on the microscopic scale.

If more than one phase is present in the porous medium, such as in oil reservoirs, where also the Richard's Equation is not valid the flow can be modeled using the Multiphase flow in Porous Media interface which couples Darcy's Law with a transport equation for the phases.

TABLE 2-1: POROUS MEDIA FLOW INTERFACES

PHYSICS INTERFACE	FLOW REGIME	EQUATION
Laminar Flow	Free Flow	Navier-Stokes Equation
Free and Porous Media Flow	Free flow and fast flow in porous media	Navier-Stokes Equation in free flow Brinkman equations in porous media
Brinkman Equations	Fast flow in porous media	Brinkman equations
Darcy's Law	Slow flow in porous media	Darcy's Law

TABLE 2-1: POROUS MEDIA FLOW INTERFACES

PHYSICS INTERFACE	FLOW REGIME	EQUATION
Richards' Equation	Variably saturated porous media	Richards' equation
Fracture Flow	Flow along surfaces of fractures	Darcy's Law
Multiphase Flow in Porous Media	Flow of more than one fluid through a porous medium	Darcy's Law Transport equation for each phase
Two-Phase Darcy's Law	Two-phase flow in porous media	Darcy's law Transport equation

Note About the Groundwater Flow Equation

In the area of hydrogeology the groundwater flow equation is commonly used to describe the groundwater flow through an aquifer. In COMSOL Multiphysics you solve equation-based models of physical processes by balancing modeled quantities, for example, mass or energy. The derivation of the groundwater flow equations starts with the mass balance in a representative elementary volume (REV). The fluxes in- and out of the REV must be in balance with the mass stored in the volume which can be expressed as:

$$q_{\rm in} = q_{\rm out} + \Delta S$$

with S denoting the storage.

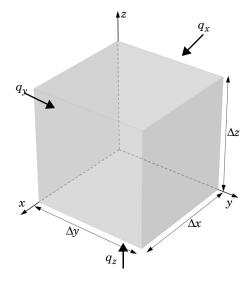


Figure 2-2: Fluxes through an elementary volume.

The flux in the x direction is:

$$(q_{x, \text{ out}} - q_{x, \text{ in}}) \Delta y \Delta z = \frac{(q_{x, \text{ out}} - q_{x, \text{ in}})}{\Delta x} \Delta x \Delta y \Delta z$$

or in differential form

$$\frac{\partial q_{x}}{\partial x} \Delta x \Delta y \Delta z$$

The flux balance in the y- and z-direction are defined accordingly and the total flux balance in the volume is

$$\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right) \Delta x \Delta y \Delta z = \Delta S$$
 (2-1)

The specific storage S_s is defined as

$$S_{\rm s} = \frac{\Delta V_{\rm w}}{\Delta h \Delta x \Delta y \Delta z}$$

where Δh denotes the change in hydraulic head which is a specific formulation for the fluid pressure (see also Pressure, Pressure Head, and Hydraulic Head Formulation). The rate of change in volume of water V_w then is

$$\frac{\Delta V_{\rm w}}{\Delta t} = -S_{\rm s} \frac{\Delta h}{\Delta t} \Delta x \Delta y \Delta z$$

together with Equation 2-1, the definition of the flux $\mathbf{q} = \rho \mathbf{u}$, and allowing for source/sink terms Q_{m} this results in the groundwater flow equation

$$S_{s} \frac{\partial h}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = Q_{m}$$
 (2-2)

In the COMSOL Multiphysics® software Equation 2-2 is formulated in terms of pressure within the Darcy's Law interface (See Pressure, Pressure Head, and Hydraulic Head Formulation). Use the Storage Model to include the Storage term on the left hand side of the equation and add a mass source to include the sink term on the right hand side.

HYDRAULIC CONDUCTIVITY

The velocity **u** in Equation 2-2 is commonly described by the formulation of Darcy law in terms of the gradient of the hydraulic head as follows:

$$\mathbf{u} = -K\nabla h \tag{2-3}$$

where K(m/s) is the hydraulic conductivity which is primarily used in hydrology applications where the fluid is water. It is related to the permeability according to

$$K = \frac{k \rho g}{\mu}$$

Note that the hydraulic conductivity is a property of both the porous matrix and the fluid, whereas the permeability describes solely the properties of the fluid.

Pressure, Pressure Head, and Hydraulic Head Formulation

In the COMSOL Multiphysics® software all equations are formulated in terms of pressure. With the Subsurface Flow Module choose to specify pressure, hydraulic head, or pressure head on the boundaries of a model. Also use pressure, hydraulic head, and pressure head during analysis and postprocessing All formulations are equivalent and can be converted into each other. Internally, when a pressure or hydraulic head is applied as boundary condition for example, the software translates it into the pressure variable.

Hydraulic head (also known as piezometric head), H(m) and pressure head, $H_{D}(m)$ relate to pressure p as

$$H_{p} = \frac{p}{\rho g}$$

$$H = H_{p} + D$$

where ρ is the fluid density, g denotes the acceleration of gravity, and D is the elevation. When defined as vertical elevation, the horizontal gradients in D equal zero and vertical gradients in D equal one. Turning off gravity effects sets the elevation D to zero, and the hydraulic head equals the pressure head.

Gravity Effects

For large-scale applications it might be necessary to take gravity effects into account. Darcy's law then applies when the gradient in hydraulic potential drives fluid movement in the porous medium. In this case Darcy's law can be written as follows:

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p + \rho \mathbf{g})$$

In this equation \mathbf{g} is the vector of gravitational acceleration. The hydraulic potential in the equation comes from the pore pressure, p, and gravity, $\rho \mathbf{g}$.

Furthermore, in the Subsurface Flow Module, g can be defined as using the elevation D according to

$$\mathbf{g} = -g\nabla D$$

where g is the magnitude of gravitational acceleration. The direction of the elevation is defined as

$$\mathbf{e}_{\mathrm{D}} = \frac{\mathbf{g}}{\|\mathbf{g}\|}$$

If a reference position r_{ref} is specified the elevation is determined using

$$D = \mathbf{e}_{\mathrm{D}} \cdot (\mathbf{r} - \mathbf{r}_{\mathrm{ref}})$$

The choice of D has a significant impact on results and the physics involved. For example, if D is the vertical coordinate z and if the flow is entirely horizontal within the xy-plane, then the gradient in D vanishes and the driving force is caused by pressure gradients alone.

Single- and Multiphase Flow Interfaces

This chapter describes the interfaces found under the Fluid Flow>Single-Phase Flow branch (\gg).

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

Under the **Fluid Flow>Multiphase Flow** branch () the following interfaces are available:

- The Phase Transport Interface
- The Phase Transport in Porous Media Interface

They are fully described in Section The Phase Transport Interfaces of the CFD Module User's Guide.

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 2-4 for links to common sections such as Discretization, Consistent Stabilization, Inconsistent Stabilization, and **Advanced Settings** sections, some of them accessed by clicking the **Show** button (**5**) 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 (<u>see</u>) 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.

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



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



Pore-Scale Flow: Application Library path Subsurface_Flow_Module/Fluid_Flow/pore_scale_flow

The Laminar Flow Interface

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

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

The equations solved by the Laminar Flow interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The Laminar Flow interface can be used for stationary and time-dependent analyses. Time-dependent studies should be used in the high-Reynolds number regime as these flows tend to become inherently unsteady.

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

SETTINGS

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

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Physics interface variables can be referred to using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

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

About the Physics Interface Label Names

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

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

Combressibility

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

When the **Incompressible flow** option (default) is selected, the incompressible form of the Navier–Stokes and continuity equations is applied. In addition, the fluid density is

evaluated at the Reference pressure level defined in this section. The Reference temperature is set to 293.15 K.

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

When the Compressible flow (Ma<0.3) option is selected, the compressible form of the Navier–Stokes and continuity equations is applied. 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.

Include Gravity

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

Also, when the **Include gravity** check box is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes are very small; otherwise, the default formulation can be used. For more information, see Gravity

Reference Values

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

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

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

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

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

DEPENDENT VARIABLES

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

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

CONSISTENT STABILIZATION

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

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

Select the **Use dynamic subgrid time scale** check box to approximate the time-scale tensor in time dependent problems from projections of weak expressions. This check box is selected by default. When not selected the actual time-step is used.

INCONSISTENT STABILIZATION

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

There is usually just one *inconsistent stabilization method* — **Isotropic diffusion**. This method is equivalent to adding a term to the diffusion coefficient in order to dampen the effect of oscillations by making the system somewhat less dominated by convection. If possible, minimize the use of the inconsistent stabilization method because by using it you no longer solve the original problem. By default, the **Isotropic** diffusion 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 underresolved problems.

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



• Numerical Stability — Stabilization Techniques for Fluid Flow

ADVANCED SETTINGS

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

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

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

The Use Block Navier-Stokes preconditioner in time dependent studies check box under Linear solvers is available when the Compressibility option is set to Incompressible flow. When this check box is selected, the default solver for time dependent study steps will use the Block Navier-Stokes preconditioner in iterative solvers for the velocity and

pressure. Using this preconditioner may result in shorter solution times for large time dependent problems with high Reynolds numbers.

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



- Theory for the Single-Phase Flow Interfaces
- Block Navier-Stokes in the COMSOL Multiphysics Reference Manual.

DISCRETIZATION

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

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

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



Flow Past a Cylinder: Application Library path

COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow

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
- Gravity
- Initial Values
- Inlet
- Line Mass Source¹
- Open Boundary
- Outlet

- Periodic Flow Condition
- Point Mass Source¹
- Pressure Point Constraint
- Symmetry
- Volume Force
- Wall



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

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

Fluid Properties

The Fluid Properties node adds the 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.

¹ A feature that may require an additional license

Temperature

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

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

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

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

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

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



Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

FLUID PROPERTIES

Density

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

Dynamic Viscosity

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

Volume Force

The **Volume Force** node specifies the volume force ${\bf F}$ 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 u** and the **Pressure** р.

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

BOUNDARY CONDITION

Select a Boundary condition for the wall.

No Slip

• Leaking Wall

Slip

No Slip

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

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

Slib

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

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_1$ 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}_{tr} . The list is per default set to Automatic from frame. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{tr} = \mathbf{0}$. If the frame moves, \mathbf{u}_{tr} becomes equal to the frame movement. \mathbf{u}_{tr} is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

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

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

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

- For 3D components, values or expressions for the **Velocity of sliding wall u**_w should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.
- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of** the tangentially moving wall $U_{\rm w}$ should be specified in 2D.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button () and selecting Advanced Physics Options in the Show More Options dialog box. The Constraints settings can be set to Default, Use pointwise constraints, Use DG constraints, or Use weak constraints. Use mixed constraints can be selected when imposing a no slip condition exactly.

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

- Apply reaction terms on can be set to Individual dependent variables (default) or All physics (symmetric). This setting is not available when **Use DG constraints** is selected.
- Select **Elemental** (default) or **Nodal** under **Constraint method**. This setting is not available for Use DG constraints or Use weak constraints.



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

Inlet

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

BOUNDARY CONDITION

The available Boundary condition options for an inlet are Velocity, Fully developed flow, 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 $\mathbf{u} = -\mathbf{n}\mathbf{U}_0$, 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.

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

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

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

FULLY DEVELOPED FLOW

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

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

• Average velocity, $U_{\rm av}$.

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

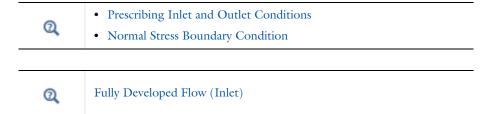
The Apply condition on each disjoint selection separately check box is selected per default. When this setting is selected, the fully developed flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The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

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

A fully developed flow boundary cannot be adjacent to any Interior Wall feature.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (5) and selecting **Advanced Physics Options.**



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, Fully developed flow, 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.

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

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

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

VELOCITY

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

FULLY DEVELOPED FLOW

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

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

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

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

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

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

A fully developed flow boundary cannot be adjacent to any Interior Wall feature.

CONSTRAINT SETTINGS

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



Prescribing Inlet and Outlet Conditions

Symmetry

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

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

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

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

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:

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

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 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

$$p = 2\mu \frac{\partial u_n}{\partial n} - \mathbf{n} \cdot \mathbf{F} \tag{3-1}$$

If $\partial u_n/\partial n$ is small, Equation 3-1 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:

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

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

for the compressible and the incompressible formulations.

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

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

If $\partial u_n/\partial n$ is small, Equation 3-2 states that $p \approx f_0$.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (**5**) 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, the orientation of the source must be specified manually (see Orientation of Source).

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

FLOW CONDITION

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

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

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

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.

Flow Continuity

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

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



About Identity and Contact Pairs

Pressure Point Constraint

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

PRESSURE CONSTRAINT

The relative pressure value is set by specifying the **Pressure** p_0 . If the reference pressure $p_{
m ref}$ 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 (5) and selecting **Advanced Physics Options.**

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

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

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

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

SOURCE STRENGTH

The source **Mass flux**, q_p should be specified. A positive value results in mass being ejected from the point into the computational domain. A negative value results in mass being removed from the computational domain.

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



Mass Sources for Fluid Flow in the COMSOL Multiphysics Reference Manual

Line Mass Source

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

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

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

SELECTION

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

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

SOURCE STRENGTH

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

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



Mass Sources for Fluid Flow in the COMSOL Multiphysics Reference Manual

Gravity

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

ACCELERATION OF GRAVITY

The Acceleration of gravity (SI unit m/s, default value $-g_{const}e_z$ in 2D axial symmetry and 3D and $-g_{const}\mathbf{e_v}$ 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
- Gravity
- Theory for the Wall Boundary Condition
- Prescribing Inlet and Outlet Conditions
- Fully Developed Flow (Inlet)
- Fully Developed Flow (Outlet)
- 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.

The Single-Phase Fluid Flow interfaces are based on the Navier-Stokes equations, which in their most general form read

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

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$
 (3-4)

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = -(\nabla \cdot \mathbf{q}) + \mathbf{K} \cdot \mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T} \Big|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla) p \right) + Q$$
 (3-5)

where

- ρ is the density (SI unit: kg/m³)
- **u** is the velocity vector (SI unit: m/s)
- p is pressure (SI unit: Pa)
- **I** is the identity matrix (unitless)
- **K** is the viscous stress tensor (SI unit: Pa)
- **F** is the volume force vector (SI unit: N/m³)
- $C_{\rm p}$ is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- **q** is the heat flux vector (SI unit: W/m²)
- Q contains the heat sources (SI unit: W/m³)
- **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

$$\mathbf{a} : \mathbf{b} = \sum_{n} \sum_{m} a_{nm} b_{nm} \tag{3-6}$$

This is sometimes referred to as the double dot product.

Equation 3-3 is the continuity equation and represents conservation of mass. Equation 3-4 is a vector equation which represents conservation of momentum. Equation 3-5 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 3-3 through Equation 3-5, constitutive relations are needed.

For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

$$\mathbf{K} = 2\mu \mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$$
 (3-7)

The dynamic viscosity, μ (SI unit: Pa·s), for a Newtonian fluid is allowed to depend on the thermodynamic state but not on the velocity field. All gases and many liquids can be considered Newtonian.

For an inelastic non-Newtonian fluid, the relationship between stress and strain rate is nonlinear, and an apparent viscosity is introduced instead of the dynamic viscosity. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions.

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

2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 3-3 and Equation 3-4 requires $\partial/\partial \phi$ to be zero. That is, there must be no gradients in the azimuthal direction. A common additional assumption is, however, that $u_{\phi} = 0$. In such cases, the ϕ -equation can be removed from Equation 3-4. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the ϕ -equation.

The default 2D axisymmetric formulation of Equation 3-3 and Equation 3-4 therefore assumes that

$$\frac{\partial}{\partial \phi} = 0$$
$$u_{\phi} = 0$$

Compressible Flow

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

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-8}$$

and the momentum equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left(\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F}$$
(3-9)

These equations are applicable for incompressible as well as for compressible flow with density and viscosity variations.

Weakly Compressible Flow

The same equations as for Compressible Flow are applied for weakly compressible flow. The only difference is that the density is evaluated at the reference pressure. The density may be a function of other quantities, in particular it may be temperature dependent.

The weakly compressible flow equations are valid for incompressible as well as compressible flow with density variations independent of the pressure.

Provided that the densities dependency pressure is specified through model inputs, the density is automatically evaluated at the reference pressure level.

The Mach Number Limit

An important dimensionless number in fluid dynamics is the Mach number, Ma, defined by

$$Ma = \frac{|\mathbf{u}|}{a}$$

where a is the speed of sound. A flow is formally incompressible when 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 3-9, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 3-8, 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 3-9 becomes vanishingly small, such as at an outflow boundary, in which case the momentum equation becomes locally hyperbolic. The number of boundary conditions to apply on the boundary then depends on the number of characteristics propagating into the computational domain. For the purely hyperbolic system, the number of characteristics propagating from the boundary into the domain changes as the Mach number passes through unity. Hence, the number of boundary conditions required to obtain a numerically well-posed system must also change. The compressible formulation of the laminar and turbulent interfaces uses the same boundary conditions as the incompressible formulation, which implies that the compressible interfaces are not suitable for flows with a Mach number larger than or equal to one. Yet, the practical Mach number limit is lower than one. The main reason is that the numerical scheme (stabilization and boundary conditions) of the Laminar Flow interface does not recognize the direction and speed of pressure waves. The fully compressible Navier-Stokes equations do, for example, start to display very sharp gradients already at moderate Mach numbers. But the stabilization for the single-phase flow interface does not necessarily capture these gradients. It is impossible to give an exact limit where the low Mach number regime ends and the moderate Mach number regime begins, but a rule of thumb is that the Mach number effects start to appear at 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, ρ is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant ρ , Equation 3-8 reduces to

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{3-10}$$

and Equation 3-9 becomes

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F}$$
 (3-11)

Provided that the densities dependency on temperature and pressure is specified through model inputs, the density is evaluated at the reference pressure level and at the reference temperature. However, if the density is a function of other quantities such as a concentration field, or if the density is specified by a user defined expression, the user has to make sure that the density is defined as constant when the incompressible flow formulation is used.

The Reynolds Number

A fundamental characteristic in analyses of fluid flow is the Reynolds number:

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.

Note that the Reynolds number can have different meanings depending on the length scale and velocity scale. To be able to compare two Reynolds numbers, they must be based on equivalent length and velocity scales.

The Fluid Flow interfaces automatically calculate the local cell Reynolds number $\operatorname{Re}^{c} = \rho |\mathbf{u}| h/(2\mu)$ using the element length h for L and the magnitude of the velocity vector u for the velocity scale U. This Reynolds number is not related to the character of the flow field, but to the stability of the numerical discretization. The risk for numerical oscillations in the solution increases as Re^c grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as: spf.cellRe).

DEFINITION

The gravity force is defined from the acceleration of gravity vector, \mathbf{g} , and the density, ρ . Under usual conditions and in Cartesian coordinates with the z-axis in the vertical direction,

$$\mathbf{g} = \begin{pmatrix} 0 \\ 0 \\ -g_{\text{const}} \end{pmatrix}.$$

When gravity is considered, a volume force equal to $\rho \mathbf{g}$ is included in the momentum equation. For example, for laminar weakly compressible flow, it reads:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) + \mathbf{F} + \rho \mathbf{g}$$
 (3-12)

Introducing a constant reference density ρ_{ref} , and assuming that **g** is homogeneous, this equation is equivalently written:

$$\begin{split} & \rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \\ & \nabla \cdot \left(-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} + \rho_{\text{ref}} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) \right) + \mathbf{F} + (\rho - \rho_{\text{ref}}) \mathbf{g} \end{split}$$
(3-13)

where \mathbf{r} is the position vector and \mathbf{r}_{ref} is an arbitrary reference position vector.

From this equation, it is convenient to define the reduced pressure which accounts for the hydrostatic pressure, $p = p - \rho_{ref} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref})$

$$\begin{split} \rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} &= \nabla \cdot \left(-\tilde{p} \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \\ \mathbf{F} + (\rho - \rho_{ref}) \mathbf{g} \end{split} \tag{3-14}$$

In Equation 3-14, the gravity force is written $(\rho-\rho_{\text{ref}})g$.

PRESSURE FORMULATION

When the relative pressure is used (default option) the interface dependent variable represents the relative pressure and the absolute pressure is defined as $p_A = p_{\rm ref} + p$. When the pressure is used to define a boundary condition (for example when p_0

defines the pressure condition at an outlet), it represents the relative pressure. Hence defining the outlet pressure as $p_{\text{hydro, approx}} = -\rho_{\text{ref}} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}})$ compensates for the gravity force for an ambient reference pressure of 0 Pa when the density is constant, there is no external force, and provided p_{ref} , \mathbf{g} and \mathbf{r}_0 are defined consistently.

When the reduced pressure is used, the interface dependent variable (named p by default) represents the reduced pressure. The absolute pressure is then defined as $p_A = p_{ref} - \rho_{ref} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref}) + p$. In this case when the pressure is used to define a boundary condition (for example to define a pressure condition at an outlet), its value corresponds to the reduced pressure. Hence, the prescribed pressure compensates for an approximate hydrostatic pressure, $p_{\text{hydro, approx}} = -\rho_{\text{ref}} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}})$ which is exact only when the density is constant and there is no external force.

PRESSURE BOUNDARY CONDITION

For an immobile fluid the momentum equation simplifies to $\nabla \cdot (p\mathbf{I}) = \mathbf{F} + \rho \mathbf{g}$ or $\nabla \cdot (-p\mathbf{I}) = \mathbf{F} + (\rho - \rho_{ref})\mathbf{g}$ depending on the pressure formulation.

For incompressible flow, assuming there are no external forces, this leads respectively to $p = -\rho_{\text{ref}} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) + p_0$ or $\tilde{p} = p_0$.

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:

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

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

$$\begin{aligned} \mathbf{u} \cdot \mathbf{n} &= 0, & \mathbf{K}_n - (\mathbf{K}_n \cdot \mathbf{n}) \mathbf{n} &= \mathbf{0} \\ \mathbf{K}_n &= \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \mathbf{n} \end{aligned}$$

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}_{tr} , \mathbf{u} in the above equations is replaced by the relative velocity $\mathbf{u}_{rel} = \mathbf{u} - \mathbf{u}_{tr}$.

POROUS SLIP

The Porous slip option, which can be chosen in the Porous treatment of no slip condition list when **Enable porous media domains** is activated, results in special treatment of **Wall** boundaries and Interior Wall boundaries adjacent to porous domains (Porous Medium feature). Namely, similar to the Navier slip boundary condition, no penetration and tangential stress conditions are applied at the wall:

$$\mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{K}_{n} - (\mathbf{K}_{n} \cdot \mathbf{n}) \mathbf{n} = -\frac{\mu}{\varepsilon_{p}} \frac{\mathbf{u}_{slip}}{y_{ps}},$$
$$\mathbf{u}_{slip} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n}) \mathbf{n}, \quad \mathbf{K}_{n} = \frac{\mu}{\varepsilon_{p}} (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) \mathbf{n}$$

Here, \mathbf{K}_{n} is the viscous wall traction, \mathbf{n} is the wall normal, \mathbf{u}_{slip} is the tangential velocity at the wall while the real no slip is assumed to be at a distance d_w (half-height of the first cell adjacent to the wall) outside the wall, and $y_{\rm ps}$ is the porous slip length. An analytical derivation of the velocity profile in the boundary layer where the pressure gradient is balanced by the sum of the Darcy term, Forchheimer drag, and a viscous term (neglecting convective terms) leads to the following expression for y_{ns} :

$$\begin{split} y_{\rm ps} &= \tilde{l} \left(\frac{1 + X_{\rm p} {\rm e}^{-\xi_{\rm p}^{c}}}{1 - X_{\rm p} {\rm e}^{-\xi_{\rm p}^{c}}} \right) \left[\left(\frac{1 + X_{\rm p} {\rm e}^{-\xi_{\rm p}^{c}}}{1 + X_{\rm p}} \right)^{2} {\rm e}^{\xi_{\rm p}^{c}} - 1 \right], \quad \xi_{\rm p} &= \frac{{\rm d}_{w}}{\tilde{l}}, \quad \tilde{l} &= \frac{l_{\rm pore}}{\sqrt{1 + 2c_{\beta}}}, \\ X_{\rm p} &= \frac{\sqrt{1 + 2c_{\beta}} - \sqrt{1 + \frac{4}{3}c_{\beta}}}{\sqrt{1 + 2c_{\beta}} + \sqrt{1 + \frac{4}{3}c_{\beta}}}, \quad c_{\beta} &= \frac{\sqrt{1 + 4c_{\rm D}} - 1}{2}, \, c_{\rm D} &= \frac{\beta_{\rm ND}}{\mu} \, \frac{\kappa^{2}}{\mu} |\nabla p - \rho {\bf g}| \end{split}$$

where $l_{\text{pore}} = \sqrt{\kappa/\varepsilon_{\text{p}}}$ is the porous length scale, $\beta_{\text{ND}} = \rho c_{\text{F}}/\sqrt{\kappa}$ is the non-Darcian coefficient (c_F is the Forchheimer coefficient), g is the gravity vector, and $\xi_{\rm p}, l, X_{\rm p}, c_{\rm \beta}, c_{\rm D}$ are intermediate variables. This formula is used when the Pressure-gradient formulation is chosen and it reads pressure-gradient at the wall. By default, the **Velocity formulation** is activated and the corresponding formula is:

$$y_{\rm ps} = \tilde{l} \ (e^{\xi_{\rm p}} - 1), \quad \xi_{\rm p} = \frac{\mathrm{d}_w}{\tilde{l}}, \quad \tilde{l} = \frac{l_{\rm pore}}{\sqrt{1 + 2c_{\beta}}},$$
$$c_{\beta} = \left[\left(\frac{\beta_{\rm ND} \kappa |\mathbf{u}_{\rm slip}|}{\mu} \frac{l_{\rm pore}}{\mathrm{d}_w} \right)^2 / 2 \right]^{1/3}$$

Although this formulation is an approximation, since it uses slip velocity at the wall to reconstruct the pressure gradient, it is rather accurate. Moreover, the influence of convective terms is partially accounted for in this formulation.

SLIDING WALL

The sliding wall option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

- In 2D, the tangential direction is unambiguously defined by the direction of the boundary, but the situation becomes more complicated in 3D. For this reason, this boundary condition has slightly different definitions in the different space dimensions.
- ullet For 2D and 2D axisymmetric components, the velocity is given as a scalar $U_{
 m w}$ and the condition prescribes

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

where $\mathbf{t} = (n_v, -n_x)$ for 2D and $\mathbf{t} = (n_z, -n_r)$ for axial symmetry.

• For 3D components, the velocity is set equal to a given vector $\mathbf{u}_{\mathbf{w}}$ projected onto the boundary plane:

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

The normalization makes **u** have the same magnitude as $\mathbf{u}_{\mathbf{w}}$ even if $\mathbf{u}_{\mathbf{w}}$ is not exactly parallel to the wall.

CONSTRAINT SETTINGS

The wall feature uses three different techniques to constraint the velocity field:

• Pointwise constraints is the standard technique to enforce strong constraints in the finite element method. The desired value of the velocity is prescribed at each node point in the mesh. Since the constraint is enforced locally at each node, only local values are affected by the constraint and the constraints are independent of each other. The solvers can therefore eliminate both the constrained degrees of freedom and the constraint force terms, effectively reducing the number of degrees of freedom being solved for.

The main advantage of pointwise constraints is that they enforce the constraint exactly pointwise. This means that they do not introduce any leakage of the velocity across the wall, unless specified. The main disadvantage of pointwise constraints is that they introduce locking effects when trying to impose a no-penetration condition for the velocity, $\mathbf{u} \cdot \mathbf{n} = 0$, on curved walls or walls with sharp corners.

- Using Weak constraints is an alternative method to prescribe the velocity. It consists on enforcing the boundary condition for the velocity via Lagrange multipliers. Their main advantage is that the Lagrange multiplier can provide an accurate representation of the reaction flux at the wall. Their main disadvantage is that they introduce extra unknowns, and are usually difficult to combine with other constraint methods on adjacent boundaries. Moreover, they may require extra constraints for the Lagrange multipliers. For more information, see Weak Constraints in the COMSOL Multiphysics Reference Manual.
- Discontinuous Galerkin (DG) constraints use a numerical flux to prescribe the velocity at the wall. They impose the constraint in a integral sense rather than pointwise, and do not suffer from the locking effects introduced by pointwise constraints when trying to prescribe a no penetration condition for the velocity. They are also better behaved when prescribing nonlinear constraints. Their main disadvantage is that the constraint is only imposed approximately, and may produce small leaks. For more information, see Discontinuous Galerkin Formulation.

The following combination of Constraint techniques can be selected in the Constraint Setting sections of Wall boundary conditions:

• Use default settings. The default settings use different constraint methods depending on whether only the normal component of the velocity is prescribed, such as in the no penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, imposed for example in Slip walls or No Slip walls using Wall Functions or Automatic Wall Treatment, or both tangential and normal components are prescribed, as is the case of No Slip walls in laminar flow.

DG constraints are used to impose the no penetration condition for Slip walls. When a No Slip condition is prescribed, pointwise constraints are used except for moving walls where DG constraints are used.

- Use Pointwise constraints.
- Use DG constraints.

- Use Weak constraints. Weak constraints are not available on Interior Walls.
- Use Mixed constraints. This option is only available when both the tangential and normal components of the velocity need to be prescribed. The velocity on the wall normal direction is imposed via pointwise constraints. The constraint for the tangential directions is relaxed, and DG constraints are used instead. This provides improved accuracy and performance when working with coarse boundary layer meshes. For more information, see Ref. 18.

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:

$$-p + 2\mu \frac{\partial u_n}{\partial n} = F_n \tag{3-15}$$

where $\partial u_n/\partial n$ is the normal derivative of the normal velocity component.

Equation 3-15 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 3-15 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 3-15, 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.

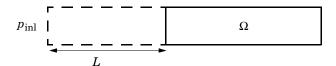
ALTERNATIVE FORMULATIONS

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

The Fully developed flow boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{inl} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$(-\mu(\nabla_{\mathbf{t}}\mathbf{u} + (\nabla_{\mathbf{t}}\mathbf{u})^T) + (p + P_{\mathrm{inl}})/2)\nabla_{\mathbf{t}}\hat{\mathbf{u}}L - P_{\mathrm{inl}}(\mathbf{n} \cdot \hat{\mathbf{u}})$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the inlet can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω . This is most notably if the flow is strongly curved just downstream of the inlet. This can for example be the case if an object is positioned just downstream of the inlet or if the adjacent boundaries are not orthogonal to the inlet. The analytical solution can in these cases be recovered by including a little bit of the inlet channel in the computational domain.

The inlet pressure, P_{inl} , must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{inl} . When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{\rm av}) \hat{P}_{\rm inl}$$

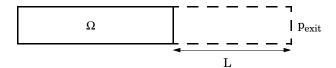
where <> denotes the average over the inlet. Since the equation for $P_{\rm inl}$ is a DAE (the equation for P_{inl} does not contain P_{inl}), it must be solved coupled to Navier–Stokes and it must be treated by a Vanka pre-smoother and post-smoother if iterative solvers are used.

The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the inlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries). So in the figure above, if the lower boundary of Ω is a no-slip wall and the top boundary is a symmetry boundary, the lower boundary of the virtually extruded channel becomes a no-slip wall and the upper boundary becomes a symmetry boundary.

Algebraic turbulence models need to additional equations or constraints. For all other turbulence models, their weak equations in the virtual inlet channel are projected onto the inlet of the computational domain. The projections are regularized to prevent the production to fall to zero, so the solutions of the projects can show slight deviation from the correct solutions close to no-slip walls.

Fully Developed Flow (Outlet)

The Fully developed flow boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{exit} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$(-\mu(\nabla_{\mathbf{f}}\mathbf{u} + (\nabla_{\mathbf{f}}\mathbf{u})^T) + (p + P_{\text{exit}})/2)\nabla_{\mathbf{f}}\hat{\mathbf{u}}L - P_{\text{exit}}(\mathbf{n} \cdot \hat{\mathbf{u}})$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the outlett can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω . The inlet pressure, P_{exit} , must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{exit} . When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{\text{av}}) \hat{P}_{\text{exit}}$$

where < > denotes the average over the inlet. Since the equation for P_{ext} is a DAE, it must be solved coupled to Navier-Stokes and it must be treated by a Vanka pre-smoother and post-smoother if iterative solvers are used.

The boundary conditions for the virtual outlet channel are inherited from the boundaries adjacent to the outlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

No Viscous Stress

For this module, and in addition to the Pressure, No Viscous Stress boundary condition, the viscous stress condition sets the viscous stress to zero:

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

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

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

$$p = 2\mu \frac{\partial u_n}{\partial n} + f_0 \tag{3-16}$$

If $\partial u_n/\partial n$ is small, Equation 3-16 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

$$\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -p_0\mathbf{n}$$
 (3-17)

$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n}$$
 (3-18)

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 3-17 or Equation 3-18 can be supplemented with a tangential velocity condition

$$\mathbf{u} \cdot \mathbf{t} = 0 \tag{3-19}$$

If so, the no-tangential-stress condition is overridden. An issue with Equation 3-17 or Equation 3-18 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

the normal stress is adjusted to keep

$$\mathbf{u} \cdot \mathbf{n} \ge 0 \tag{3-21}$$

Equation 3-20 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 3-20 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

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

$$\mathbf{n}^{T} \left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T})\right)\mathbf{n} = -\hat{p}_{0}$$

$$\hat{p}_{0} \geq p_{0}$$
(3-22)

together with the tangential condition in Equation 3-19, or, a general flow direction is prescribed.

$$\begin{split} \mathbf{r}_{\mathbf{u}}^T & \Big(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I} \Big) \mathbf{n} = -\hat{p}_0(\mathbf{r}_{\mathbf{u}}\cdot\mathbf{n}) \\ & \mathbf{r}_{\mathbf{u}}^T (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) \mathbf{n} = -\hat{p}_0(\mathbf{r}_{\mathbf{u}}\cdot\mathbf{n}) \\ & \hat{p}_0 \geq p_0 \\ & \mathbf{u} - (\mathbf{u}\cdot\mathbf{r}_{\mathbf{u}})\mathbf{r}_{\mathbf{u}} = \mathbf{0}, \ \mathbf{r}_{\mathbf{u}} = \frac{\mathbf{d}_{\mathbf{u}}}{\left\|\mathbf{d}_{\mathbf{u}}\right\|} \end{split} \tag{3-23}$$

The ">" option is used with suppress backflow to have $\mathbf{u} \cdot \mathbf{n} \leq 0$ or $\mathbf{u} \cdot \mathbf{r}_{\mathbf{u}} \geq 0$.

For incompressible single-phase flow, it is also allowed to specify the total pressure, p_{tot} , instead of the static pressure, p_{stat} , on inlet and outlet boundaries. It is more useful, for example, in pump applications. The pressure is then prescribed at the boundaries using Bernoulli's principle,

$$p = p_{\text{stat}} = p_{\text{tot}} - \frac{1}{2} \rho |\mathbf{u}|^2$$
 (3-24)

The equation is imposed with two options: Average and Pointwise.

In the first option, p_{stat} is prescribed by:

$$\mathbf{n}^{T}(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{T}))\mathbf{n} = \mathbf{n}^{T}(-p_{\text{obs}}\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{T}))\mathbf{n}$$
(3-25)

where p_{tot} and $|\mathbf{u}|^2$ are averaged over the boundaries using the aveop operator:

$$p_{\text{stat}} = \text{aveop}(p_{\text{tot}}) - \frac{1}{2} \rho \cdot \text{aveop}(|\mathbf{u}|^2)$$

For the second option, Equation 3-24 is prescribed pointwise.

See Inlet, Outlet, Open Boundary, and No Viscous Stress for the individual node settings. Note that some modules have additional theory sections describing options available with that module.

There are two types of mass sources in a Single-Phase Flow interface: point sources and line sources.



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

POINT SOURCE

A point source is theoretically formed by taking a mass injection/ejection, \dot{Q} (SI unit: $kg/(m^3 \cdot s)$, in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_{\rm p}$ (SI unit: kg/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q} = \dot{q}_{p} \tag{3-26}$$

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

$$\dot{q}_{\rm p}{\rm test}(p)$$

is added to a point in the geometry. As can be seen from Equation 3-26, \hat{Q} must tend to plus or minus infinity as δV tends to zero. This means that in theory the pressure also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 3-26 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 Q (SI unit: kg/(m³·s)), located within a tube with cross-sectional area δS and then letting δS tend to zero, while keeping the total mass flux per unit length constant. Given a line source strength, \dot{q}_1 (SI unit: kg/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_1 \tag{3-27}$$

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

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

is added to lines in 3D or to points in 2D (which represent cut-through views of lines). Line sources can also be added to the axisymmetry line in 2D axisymmetry components. It cannot, however, be added to geometrical lines in 2D because they represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.



For feature node information, see Line Mass Source and Point Mass Source in the COMSOL Multiphysics Reference Manual.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, these shared physics nodes are renamed as follows:



- The Line Mass Source node is available as two nodes, one for the fluid flow (Fluid Line Source) and one for the species (Species Line Source).
- The **Point Mass Source** node is available as two nodes, one for the fluid flow (Fluid Point Source) and one for the species (Species Point Source).

Numerical Stability — Stabilization Techniques for Fluid Flow

The momentum equation (Equation 3-9 or Equation 3-11) is a (nonlinear) convection-diffusion equation. Such equations can easily become unstable if discretized using the Galerkin finite element method. Stabilized finite element methods are usually necessary in order to obtain physical solutions. The stabilization settings are found in the main Fluid Flow interface features. To display this section, click the Show More Options button (5) and select Stabilization in the Show More **Options** dialog box.

There are three types of stabilization methods available for Navier-Stokes streamline diffusion, crosswind diffusion, and isotropic diffusion. Streamline diffusion and crosswind diffusion are consistent stabilization methods, whereas isotropic diffusion is an inconsistent stabilization method.

For optimal functionality, the exact weak formulations of and constants in the streamline diffusion and crosswind diffusion methods depend on the order of the shape functions (basis functions) for the elements. The values of constants in the streamline diffusion and crosswind diffusion methods follow Ref. 5 and Ref. 6.

STREAMLINE DIFFUSION

For strongly coupled systems of equations, the streamline diffusion method must be applied to the system as a whole rather than to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 8) and were later extended to Galerkin least-squares (GLS) applied to the Navier-Stokes equations (Ref. 9). This is the streamline diffusion formulation that COMSOL Multiphysics supports. The time-scale tensor is the diagonal tensor presented in Ref. 10.

The time-scale tensors for time-dependent problems should in theory depend on a time-scale that many references just set to the time-step taken by the time-solver, Δt (see for example Ref. 9 and Ref. 10). This simple approach does not, however, necessarily reflect on the actual time-scales in the physics. A typical example is reacting flows where the time step is often guided by fast reactions, while the flow develops relatively slowly. The COMSOL Multiphysics software can therefore replace Δt^2 in the time-scale tensor with measures of type $(1/(\Delta t)^2)^{-1}$, which are calculated from projections of weak expressions in a fashion similar to those in Ref. 11. These measures of the time scale are used when **Use dynamic subgrid time scale** check box is selected. Streamline diffusion is active by default because it is necessary when convection is dominating the flow.

The governing equations for incompressible flow are subject to the Babuška–Brezzi condition, which states that the shape functions (basis functions) for pressure must be of lower order than the shape functions for velocity. If the incompressible Navier-Stokes equations are stabilized by streamline diffusion, it is possible to use equal-order interpolation. Hence, streamline diffusion is necessary when using first-order elements for both velocity and pressure. This applies also if the model is solved using geometric multigrid (either as a solver or as a preconditioner) and at least one multigrid hierarchy level uses linear Lagrange elements.

CROSSWIND DIFFUSION

Crosswind diffusion can also be formulated for systems of equations, and when applied to the Navier-Stokes equations it becomes a shock-capturing operator. COMSOL Multiphysics supports the formulation in Ref. 9 with a shock-capturing viscosity of the Hughes–Mallet type Ref. 8.

Incompressible flows do not contain shock waves, but crosswind diffusion is still useful for introducing extra diffusion in sharp boundary layers and shear layers that otherwise would require a very fine mesh to resolve.

Crosswind diffusion is active by default as it makes it easier to obtain a solution even if the problem is fully resolved by the mesh. Crosswind diffusion also enables the iterative solvers to use inexpensive presmoothers. If crosswind diffusion is deactivated, more expensive preconditioners must be used instead.

ISOTROPIC DIFFUSION

Isotropic diffusion adds diffusion to the Navier-Stokes equations. Isotropic diffusion significantly reduces the accuracy of the solution but does a very good job at reducing oscillations. The stability of the continuity equation is not improved.



Numerical Stabilization and Iterative in the COMSOL Multiphysics Reference Manual.

Solvers for Laminar Flow

The Navier-Stokes equations constitute a nonlinear equation system. A nonlinear solver must hence be applied to solve the problem. The nonlinear solver iterates to reach the final solution. In each iteration, a linearized version of the nonlinear system is solved using a linear solver. In the time-dependent case, a time marching method must also be applied. The default suggestions for each of these solver elements are discussed below.

NONLINEAR SOLVER

The nonlinear solver method depends on if the model solves a stationary or a time-dependent problem.

Stationary Solver

In the stationary case, a fully coupled, damped Newton method is applied. The initial damping factor is low since a full Newton step can be harmful unless the initial values are close to the final solution. The nonlinear solver algorithm automatically regulates the damping factor in order to reach a converged solution.

For advanced models, the automatically damped Newton method might not be robust enough. A pseudo time-stepping algorithm can then be invoked. See Pseudo Time Stepping for Laminar Flow Models.

Time-Dependent Solver

In the time-dependent case, the initial guess for each time step is (loosely speaking) the previous time step, which is a very good initial value for the nonlinear solver. The automatic damping algorithm is then not necessary. The damping factor in the Newton method is instead set to a constant value slightly smaller than one. Also, for the same reason, it suffices to update the Jacobian once per time step.

It is seldom worth the extra computational cost to update the Jacobian more than once per time step. For most models it is more efficient to restrict the maximum time step or possibly lower the damping factor in the Newton method.

LINEAR SOLVER

The linearized Navier–Stokes equation system has saddle point character, unless the density depends on the pressure. This means that the Jacobian matrix has zeros on the diagonal. Even when the density depends on the pressure, the equation system effectively shares many numerical properties with a saddle point system.

For small 2D and 3D models, the default solver suggestion is a direct solver. Direct solvers can handle most nonsingular systems and are very robust and also very fast for small models. Unfortunately, they become slow for large models and their memory requirement scales as somewhere between $N^{1.5}$ and N^2 , where N is the number of degrees of freedom in the model. The default suggestion for large 2D and 3D models is therefore the iterative GMRES solver. The memory requirement for an iterative solver optimally scales as N.

GMRES is accelerated by a multigrid method, per default the smoothed aggregation algebraic multigrid (SAAMG) method. The cost of SAAMG is typically very low compared to the number of GMRES iterations necessary if no multigrid method is used. As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, the geometric multigrid (GMG) method requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared-memory computations with many cores. When the default linear solver is GMRES, an optional, but deactivated, linear solver node is available where GMRES is accelerated by GMG.

Multigrid methods need smoothers, but the saddle point character of the linear system restricts the number of applicable smoothers. The choices are further restricted by the anisotropic meshes frequently encountered in fluid-flow problems. The efficiency of the smoothers is highly dependent on the numerical stabilization. Iterative solvers perform at their best when both Streamline Diffusion and Crosswind Diffusion are active.

The default smoother for P1+P1 elements is SCGS. This is an efficient and robust smoother specially designed to solve saddle point systems on meshes that contain anisotropic elements. The SCGS smoother works well even without crosswind diffusion. SCGS can sometimes work for higher-order elements, especially if **Method** in the SCGS settings is set to **Mesh element lines**. But there is no guarantee for this, so the

default smoother for higher order elements is an SOR Line smoother. SOR Line handles mesh anisotropy but does not formally address the saddle point character. It does, however, function in practice provided that streamline diffusion and crosswind diffusion are both active.

A different kind of saddle point character can arise if the equation system contains ODE variables. Some advanced boundary conditions can add equations with such variables. These variables must be treated with the Vanka algorithm. SCGS includes an option to invoke Vanka. Models with higher-order elements must apply SCGS or use the Vanka smoother. The latter is the default suggestion for higher-order elements, but it does not work optimally for anisotropic meshes.

TIME-DEPENDENT SOLVERS

The default time-dependent solver for Navier-Stokes is the BDF method with maximum order set to two. Higher BDF orders are not stable for transport problems in general nor for Navier-Stokes in particular.

BDF methods have been used for a long time and are known for their stability. However, they can have severe damping effects, especially the lower-order methods. Hence, if robustness is not an issue, a model can benefit from using the generalized- α method instead. Generalized- α is a solver which has properties similar to those of the second-order BDF solver but it is much less diffusive.

Both BDF and generalized- α are per default set to automatically adjust the time step. While this works well for many models, extra efficiency and accuracy can often be gained by specifying a maximum time step. It is also often beneficial to specify an initial time step to make the solver progress smoothly in the beginning of the time series.

In the COMSOL Multiphysics Reference Manual:



- Time-Dependent Solver
- Multigrid, Direct, Iterative, SCGS, SOR Line, and Vanka
- Stationary Solver

Pseudo Time Stepping for Laminar Flow Models

A stationary formulation has per definition no time derivatives and Equation 3-11 reduces to:

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F}$$
(3-28)

Solving Equation 3-28 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 3-28:

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

where $\Delta \tilde{t}$ 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 Δt can be chosen individually for each element based on the local CFL number:

$$\Delta \tilde{t} = CFL_{loc} \frac{h}{|\mathbf{u}|}$$

where h is the mesh cell size. A small CFL number means a small time step. It is practical to start with a small CFL number and gradually increase it as the solution approaches steady state.

If the automatic expression for CFL_{loc} is set to the built-in variable CFLCMP, then the automatic setting suggests a PID regulator for the pseudo time step in the default solver. The PID regulator starts with a small CFL number and increases CFL_{loc} as the solution comes closer to convergence.

The default manual expression is

$$1.3^{\min(\text{niterCMP}, 9)} + \\ if(\text{niterCMP} > 20, 9 \cdot 1.3^{\min(\text{niterCMP} - 20, 9)}, 0) + \\ if(\text{niterCMP} > 40, 90 \cdot 1.3^{\min(\text{niterCMP} - 40, 9)}, 0)$$

The variable niterCMP is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. CFL_{loc} starts at 1.3 and increases by 30% each iteration until it reaches $1.3^9 \approx 10.6$. It remains there until iteration number 20 at which it starts to increase until it reaches approximately 106. A final increase after iteration number 40

then takes it to 1060. Equation 3-29 can, for some advanced flows, increase CFL_{loc} too slowly or too quickly. CFL_{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 nonzero 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. 15.

In particular, the SIPG formulation includes a penalty parameter that must be large enough for the formulation to be coercive. The higher the value, the better the boundary condition is fulfilled, but a too high value results in an ill-conditioned equation system. The penalty parameter in COMSOL Multiphysics is implemented according to Ref. 16.

Particle Tracing in Fluid Flow

The Particle Tracing Module is available to assist with these types of modeling problems.

It is possible to model particle tracing with COMSOL Multiphysics provided that the impact of the particles on the flow field is negligible. First compute the flow field, and then, as an analysis step, calculate the motion of the particles. The motion of a particle is defined by Newton's second law

$$m\frac{d^2\mathbf{x}}{dt^2} = \mathbf{F}\left(t, \mathbf{x}, \frac{d\mathbf{x}}{dt}\right)$$

where \mathbf{x} is the position of the particle, m the particle mass, and \mathbf{F} is the sum of all forces acting on the particle. Examples of forces acting on a particle in a fluid are the drag force, the buoyancy force, and the gravity force. The drag force represents the force that a fluid exerts on a particle due to a difference in velocity between the fluid and the particle. It includes the viscous drag, the added mass, and the Basset history term. Several empirical expressions have been suggested for the drag force. One of those is the one proposed by Khan and Richardson (Ref. 13). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

$$Re_p = \frac{|\mathbf{u} - \mathbf{u}_p| 2r\rho}{\mu}$$

where \mathbf{u} is the velocity of the fluid, \mathbf{u}_p the particle velocity, r the particle radius, ρ the fluid density, and μ the dynamic viscosity of the fluid. The empirical expression for the drag force according to Khan and Richardson is

$$\mathbf{F} = \pi r^2 \, \rho |\mathbf{u} - \mathbf{u}_p| (\mathbf{u} - \mathbf{u}_p) [1.84 \,\text{Re}_p^{-0.31} + 0.293 \,\text{Re}_p^{0.06}]^{3.45}$$

The model *Flow Past a Cylinder* (Application Library path COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow) demonstrates how to add and set up particle tracing in a plot group using the Particle Tracing with Mass node. It uses the predefined Khan-Richardson model for the drag force and neglects gravity and buoyancy forces.

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Porous Media and Subsurface Flow Interfaces

This chapter has information about the physics interfaces found under the Fluid Flow>Porous Media and Subsurface Flow branch (). It contains physics interfaces for the following sets of equations that apply under different conditions:

- The Darcy's Law Interface describes low-velocity flows of one or more fluids.
- The Richards' Equation Interface governs the wetting and drying of rocks or soils.
- The Two-Phase Darcy's Law Interface describes two-phase fluid movement through interstices in a porous medium. An extra equation is computed to calculate the saturation transport.
- The Multiphase Flow in Porous Media Interface which combines low velocity flow with phase transport of multiple immiscible phases in a porous medium is described in Chapter Multiphysics Interfaces and Couplings.
- The Fracture Flow Interface is a variant of Darcy's law that defines the flow along the interior boundaries representing fractures within a porous or solid medium.
- The Brinkman Equations Interface is for porous media high-velocity flows.
- The Free and Porous Media Flow Interface combines free flow adjacent to porous domains.
- The Laminar Flow and Creeping Flow Interfaces use the *Navier-Stokes* equations (in which the inertia term is neglected in case of Creeping Flow) to

describe free flows within a river or well, for example. The Laminar Flow Interface is available with all COMSOL licenses.

With Darcy's law and Richards' equation, COMSOL Multiphysics solves for pressure and has physics interfaces for pressure head and hydraulic head. Set up these equations for single or multiple fluids. The physics interfaces can be coupled to other physics interfaces to describe poroelasticity, convection of heat- and density-driven flows, solute transfer, and electromagnetic forces, to name a few.

In this chapter you will find the following sections:

- · Darcy's Law:
 - Theory for the Darcy's Law Interface
 - The Darcy's Law Interface
- Richards' Equation:
 - Theory for the Richards' Equation Interface
 - The Richards' Equation Interface
- Two-Phase Darcy's Law:
 - Theory for the Two-Phase Darcy's Law Interface
 - The Two-Phase Darcy's Law Interface
- · Fracture Flow:
 - Theory for the Fracture Flow Interface
 - The Fracture Flow Interface
- Brinkman Equations:
 - Theory for the Brinkman Equations Interface
 - The Brinkman Equations Interface
- Free and Porous Media Flow:
 - Theory for the Free and Porous Media Flow Interface
 - The Free and Porous Media Flow Interface

Theory for the Darcy's Law Interface

The Darcy's Law Interface theory is described in this section:

- About Darcy's Law
- Darcy's Law Equation Formulation
- Storage Model
- Average Linear Velocity
- References for the Darcy's Law Interface

About Darcy's Law

In a porous medium, the global transport of momentum by shear stresses in the fluid is often negligible, because the pore walls impede momentum transport to the fluid outside the individual pores. A detailed description, down to the resolution of every pore, is not practical in most applications. A homogenization of the porous and fluid media into a single medium is a common alternative approach. Darcy's law together with the continuity equation and equation of state for the pore fluid (or gas) provide a complete mathematical model suitable for a wide variety of applications involving porous media flows, for which the pressure gradient is the major driving force.

Darcy's law describes fluid movement through interstices in a porous medium. Because the fluid loses considerable energy to frictional resistance within pores, flow velocities in porous media are very low. The Darcy's Law interface can be applied to small-scale tasks in chemical engineering as well as to large-scale geophysical or hydrological tasks such as water moving in an aquifer or stream bank, oil migrating to a well, and even magma rising through the earth to a chamber in a volcano (see Ref. 1, Ref. 2, Ref. 3, and Ref. 4). Also set up multiple Darcy's Law interfaces to model multiphase flows involving more than one mobile phase.

Darcy's law describes flow in porous media driven by gradients in the hydraulic potential field, which has units of pressure. For many applications it is convenient to represent the total hydraulic potential or the pressure and the gravitational components with equivalent heights of fluid or head. Division of potential by the fluid weight can simplify modeling because units of length make it straightforward to compare to many physical data. Consider, for example, fluid levels in wells, stream heights, topography, and velocities. The physics interface also supports specifying

boundary conditions and result evaluation using hydraulic head and pressure head. In the physics interface, pressure is always the dependent variable.

Darcy's Law — Equation Formulation

Darcy's law states that the velocity field is determined by the pressure gradient, the fluid viscosity, and the structure of the porous medium:

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{4-1}$$

In this equation, **u** is the Darcy's velocity or specific discharge vector (SI unit: m/s); κ is the permeability of the porous medium (SI unit: m²); μ is the fluid's dynamic viscosity (SI unit: Pa·s); p is the pore pressure (SI unit: Pa) and ρ is the density of the fluid (SI unit: kg/m³).

The above equation formulation is called linear Darcy law. The
applicability of this formulation is discussed in the chapter About
Darcian and Non-Darcian Flow in the Porous Media Flow Module
User's Guide.



- Permeability can be defined in different ways, either directly or based on predefined permeability models. These are described in detail in the chapter Permeability Models.
- For a detailed overview of the permeability models available in each product visit https://www.comsol.com/products/specifications/.

The Darcy's Law interface combines Darcy's law with the continuity equation

$$\frac{\partial}{\partial t}(\rho \varepsilon_{\rm p}) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m} \tag{4-2}$$

In the above equation, ρ is the fluid density (SI unit: kg/m³), ε_p is the porosity, and $Q_{\rm m}$ is a mass source term (SI unit: kg/(m³·s)). Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

For large-scale applications it might be necessary to take gravity effects into account. Darcy's law then applies when the gradient in hydraulic potential drives fluid movement in the porous medium. Darcy's law then has the form:

$$\mathbf{u} = -\frac{\kappa}{u}(\nabla p + \rho \mathbf{g}) \tag{4-3}$$

• See the section Gravity Effects in the Subsurface Flow Module User's Guide.



- Note that gravity effects are only included in some modules. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.
- Gravity effects are not active by default. Select the check box Include **gravity** to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

Storage Model

Inserting Darcy's law (Equation 4-1) into the continuity equation produces the generalized governing equation

$$\frac{\partial}{\partial t}(\rho \varepsilon_{\rm p}) + \nabla \cdot \rho \left[-\frac{\kappa}{\mu}(\nabla p) \right] = Q_{\rm m} \tag{4-4}$$

Represent this equation fully in COMSOL Multiphysics because relationships between density or permeability can be freely specified, for example, and pressure, temperature, concentration, and so on.

Expand the time-derivative term in Equation 4-4

$$\frac{\partial}{\partial t}(\rho \varepsilon_{p}) = \varepsilon_{p} \frac{\partial \rho}{\partial t} + \rho \frac{\partial \varepsilon_{p}}{\partial t}$$

Define the porosity and the density as functions of the pressure, and apply the chain rule

$$\varepsilon_{\mathbf{p}} \frac{\partial \rho}{\partial t} + \rho \frac{\partial \varepsilon_{\mathbf{p}}}{\partial t} = \varepsilon_{\mathbf{p}} \frac{\partial \rho}{\partial p} \frac{\partial p}{\partial t} + \rho \frac{\partial \varepsilon_{\mathbf{p}}}{\partial p} \frac{\partial p}{\partial t}$$

Insert the definition of fluid compressibility $\chi_f = (1/\rho)(\partial \rho/\partial p)$ to the right-hand side and rearrange to arrive at

$$\frac{\partial(\rho\varepsilon_{\rm p})}{\partial t} = \rho \left(\varepsilon_{\rm p}\chi_{\rm f} + \frac{\partial\varepsilon_{\rm p}}{\partial p}\right) \frac{\partial p}{\partial t} = \rho S \frac{\partial p}{\partial t}$$

Using this relation, the generalized governing equation (Equation 4-4) takes the following form:

$$\rho S \frac{\partial p}{\partial t} + \nabla \cdot \rho \left[-\frac{\kappa}{\mu} (\nabla p) \right] = Q_{\rm m} \tag{4-5}$$

In this equation, S is the storage coefficient (SI unit: 1/Pa), which can be interpreted as the weighted compressibility of the porous material and the fluid. The storage S can be an expression involving results from a solid-deformation equation or an expression involving temperatures and concentrations from other analyses. The Darcy's Law interface implements Equation 4-5 in the **Porous Medium** node, which explicitly includes different storage models to choose from, such as *linearized storage* which defines S (SI unit: 1/Pa) using the compressibility of fluids χ_f and of the porous matrix χ_p :

$$S = \varepsilon_{p} \chi_{f} + (1 - \varepsilon_{p}) \chi_{p},$$

or the poroelastic storage where

$$S = \varepsilon_{p} \chi_{f}$$
.



The Storage Model node is only available for the Subsurface Flow Module and the Porous Media Flow Module. For a detailed overview of the functionality available in each product visit

https://www.comsol.com/products/specifications/.

Average Linear Velocity

Because fluids typically occupy only 10% to 50% of a porous medium, it follows that velocities within the pore channels exceed the Darcy velocity, \mathbf{u} , on the order of two to ten times. For clarity, the physics interface includes the average linear velocity within the pores, \mathbf{u}_{α} , (also termed the seepage velocity) defined as $\mathbf{u}_{\alpha} = \mathbf{u}/\epsilon_p$, where ϵ_p is the porosity.

References for the Darcy's Law Interface

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The Darcy's Law Interface

The Darcy's Law (dl) interface (🔊), found under the Porous Media and Subsurface Flow branch () when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. Set up multiple Darcy's Law interfaces to model multiphase flows involving more than one mobile phase. The Darcy's Law interface can be used for stationary and time-dependent analyses.

The main feature is the **Porous Medium** Properties node, which provides interfaces for defining the fluid material and the porous matrix properties.

When this physics interface is added, the following default nodes are also added in the Model Builder — Porous Medium, No Flow (the default boundary condition), and Initial **Values.** Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click Darcy's Law to select physics features from the context menu.

SETTINGS

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

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>. <variable name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is d1.

PHYSICAL MODEL

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

GRAVITY EFFECTS

By default there are no gravity effects added to Darcy's Law interface. Select the check box **Include gravity** to activate the acceleration of gravity. When this check box is selected a global **Gravity** feature node is shown in the interface model tree.

Enter a value for the acceleration of gravity. The default value g const is the predefined standard acceleration of gravity on Earth.



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

DISCRETIZATION

To display all settings available in this section, click the **Show More Options** button (**5**) and select Advanced Physics Options in the Show More Options dialog box.

You can choose the order of the shape functions used for the pressure variable solved by the Darcy's Law interface. The default shape functions are **Quadratic** Lagrange.

The **Compute boundary fluxes** 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, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

Also, the Apply smoothing to boundary fluxes 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.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure**. The name can be changed but the names of fields and dependent variables must be unique within a model.



- Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface
- Theory for the Darcy's Law Interface
- Physical Constants in the COMSOL Multiphysics Reference Manual
- Species Transport in the Gas Diffusion Layers of a PEM: Application Library path

Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pem_gdl_species_transport _2d



- Steam Reformer: Application Library path Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/ steam_reformer
- Terzaghi Compaction: Application Library path Subsurface_Flow_Module/Flow_and_Solid_Deformation/terzaghi_compacti on

Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface

The Darcy's Law Interface has the following domain, boundary, edge, point, and pair nodes, these nodes are available from the **Physics** ribbon toolbar (Windows users), Physics context menu (Mac or Linux users), or right-click to access the context menu (all users).

DOMAIN

• Porous Medium

Gravity

• Cross Section

• Initial Values

Mass Source

Thickness

• Porous Electrode Coupling

• Unsaturated Porous Medium

Note that some features are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/).

BOUNDARY, EDGE, AND POINT

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

• Atmosphere/Gauge

• Electrode Surface Coupling

• Flux Discontinuity • Fracture Flow

• Hydraulic Head

Inlet

• Interior Wall

• Line Mass Source

Mass Flux

• No Flow

Outlet

• Pervious Layer

• Point Mass Source

• Precipitation

• Pressure

• Pressure Head

Reaction Coefficients¹

• Symmetry

• Thin Barrier

Note that some features are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/)!

The relevant physics interface condition at interior boundaries is continuity:

$$\boldsymbol{n}\cdot(\rho_1\boldsymbol{u}_1\text{-}\rho_2\boldsymbol{u}_2) = 0$$

The continuity boundary condition ensures that the pressure and mass flux are continuous. In addition, the Pressure boundary condition is available on interior boundaries.

¹ This node is described for the Transport of Diluted Species Interface

The continuity boundary condition provides continuity for the pressure and mass flux. In addition, the following boundary conditions are available on interior boundaries:

• Pressure

• Pressure Head

Hydraulic Head

· Interior Wall

• Pervious Layer

Flux Discontinuity

• Fracture Flow

• Thin Barrier



In general, to add a node, go to the Physics toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.



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



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

Porous Medium

The **Porous Medium** node adds the equations for modeling flow through porous domains. By default these are Equation 4-6 and Equation 4-7 (excluding any mass sources).

$$\frac{\partial}{\partial t}(\varepsilon_{p}\rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{\mathrm{m}}$$
 (4-6)

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{4-7}$$

For a steady-state problem the first term in Equation 4-6 disappears. When Gravity is active Equation 4-7 is of the following form:

$$\mathbf{u} = -\frac{\kappa}{\mu} (\nabla p + \rho \mathbf{g}) \tag{4-8}$$

The Porous Medium feature has two default subfeatures — the Fluid subfeature where the fluid density $\rho(SI \text{ unit: kg/m}^3)$ and dynamic viscosity $\mu(SI \text{ unit: Pa·s})$ are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m^2) and porosity ε_p (dimensionless) are specified.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the Global coordinate system, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or Hydraulic conductivity (in the Porous Matrix subnode) should be set according to the coordinate system selected in this section.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- Darcian flow (default) defines a linear relationship using Equation 4-6 and Equation 4-7.
- Non-Darcian flow defines a nonlinear relationship using Equation 4-6 and

$$\nabla p = -\frac{\mu}{\kappa} \mathbf{u} - \beta \rho |\mathbf{u}| \mathbf{u}$$

where the nonlinear parameter β (SI unit: 1/m) is further specified in the Porous Matrix subfeature.

STORAGE MODEL

Equation 4-6 can also be formulated with respect to a storage term.

$$\rho S \frac{\partial p}{\partial t} + \nabla \cdot \rho \left[-\frac{\kappa}{\mu} (\nabla p) \right] = Q_{\rm m} \tag{4-9}$$

The storage coefficient S can be interpreted as the weighted compressibility of the porous material and the fluid. Define the time dependent storage term by selecting one of the following options from the drop-down menu:

- From density and porosity (default), uses the formulation of Equation 4-6
- **Linearized storage**, where the following linear equation is used to define the storage:

$$S = \varepsilon_{p} \chi_{f} + (1 - \varepsilon_{p}) \chi_{p}$$

- Poroelastic storage, where $S = \varepsilon_p \chi_f$
- Quasistatic, where the storage term is set to zero
- User defined to directly specify the storage coefficient S

Note that the option to choose a different Flow model and Storage model is only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.



- Porous Material in the COMSOL Multiphysics Reference Manual
- About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide
- Storage Model in the Subsurface Flow Module User's Guide

Fluid

This node defines the material properties of the fluid of the Porous Medium or Unsaturated Porous Medium parent node. The fluid can be specified as general gas or liquid or as an ideal gas.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

The available options for the Fluid type are Gas/Liquid (default) or Ideal gas. The selection determines how the density and compressibility of the fluid are set. The latter is only required if a poroelastic or linearized storage model has been selected in the parent Porous Medium node. For all fluid types specify the dynamic viscosity μ (SI unit: Pa·s).

Gas/Liauid

This option specifies the **Density** and the **Compressibility** for a general gas or liquid.

Ideal Gas

For Ideal gas it uses the ideal gas law to describe the fluid. In this case, specify the thermodynamics properties. Select a Gas constant type — Specific gas constant ${\cal R}_s$ (the default) or Mean molar mass M_n (SI unit: $J/(\text{mol}\cdot K)$). For Mean molar mass the universal gas constant $R = 8.314 \text{ J/(mol \cdot \text{K})}$ is used as the built-in physical constant. For both properties, the defaults use values From material. For User defined enter another value or expression.

If required by a Storage Model, the Compressibility of the ideal gas is calculated as $\chi_{\rm f} = 1/p_{\rm A}$ with the absolute pressure $p_{\rm A}$ (Pa).

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium or Unsaturated Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The default Porosity $\varepsilon_{\rm p}$ of the solid matrix is taken From material. In a Porous Material node, the porosity is defined as follows:

$$\varepsilon_{\rm p} = 1 - \sum_{i} \theta_{{\rm s}i} - \sum_{i} \theta_{{\rm imf}i}$$

where θ_{si} and θ_{imfi} are the porosities of the **Solid** and **Immobile Fluids** subnodes under the Porous Material node. See Porous Material in the COMSOL Multiphysics Reference Manual for more information.

Select **User defined** to enter a value or expression for $\varepsilon_{\rm p}$.

If required by a Storage model in the parent node, specify the Effective compressibility of the porous matrix. The default value is $\chi_p = 10^{-4} Pa$.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Which options are available depends on the **Flow model** setting in the parent node. Note that for the Unsaturated Porous Medium parent node only the Darcian Flow models are available.

Darcian Flow

If Darcian flow is selected in the parent Porous medium node, select between the following options for the Permeability model:

- Select Permeability (default) to define the permeability of the porous matrix. The default **Permeability** $\kappa(SI \text{ unit: } m^2)$ uses the value **From material**, as defined by the Porous material. For User defined select Isotropic to define a scalar value or Diagonal or **Symmetric** to define a tensor value.
- Select Hydraulic conductivity or define a combination of fluid permeability and dynamic viscosity. For Hydraulic conductivity K(SI unit: m/s) select Isotropic to define a scalar value or Diagonal or Symmetric to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter** $d_{\rm p}$ (SI unit: m), the default value is 0.5 mm.

Non-Darcian Flow

Select between the following options for the Permeability model:

- For Forchheimer, the default Permeability $\kappa(\mathrm{SI~unit:m^2})$ uses the value From material, as defined by the Porous material list. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.
- If **Ergun** is selected, enter the mean **Particle diameter** $d_{\rm p}$ (default value: 0.5 mm).
- For Burke-Plummer, specify the mean Particle diameter $d_{\rm p}$ (default value: 0.5 mm).
- For Klinkenberg, the default Permeability κ_{∞} (SI unit: m²) uses the value From material. Enter the Klinkenberg parameter b_K . Its default value is 1e3 Pa.

Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit

https://www.comsol.com/products/specifications/.



- About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide
- Permeability Models in the Porous Media Flow Module User's Guide

RETENTION MODEL

For an Unsaturated Porous Medium select between the following options for the retention model:

- van Genuchten, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants α (default is 1, and the SI unit is 1/m), n (default is 2), and I (default is 0.5). The constitutive parameter m is equal to 1-1/n.
- **Brooks and Corey** to use the retention model according to the Brooks and Corey relationships.
- User defined to use a different retention model. Enter user defined expressions for the Effective saturation S_e , the Liquid volume fraction θ_l . The default is ϵ_p (the porosity variable). Specify the Specific moisture capacity C_{m} (SI unit: $1/\mathrm{m}$). The default is 0 (1/m). Enter an expression for th Relative permeability $\kappa_r\!$. The default is 1.

If there is a residual volume of liquid that cannot move through the pore network, also enter a a value between 0 and 1 for the Residual liquid volume fraction θ_r . The default value is 0.



Retention and Permeability Relationships in the Subsurface Flow Module User's Guide

Mass Source

The Mass Source node adds a mass source $Q_{\rm m}$, which appears on the right-hand side of the Darcy's Law equation (Equation 4-6).

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_{\mathrm{m}} \tag{4-10}$$

For The Fracture Flow Interface — which is available for the Subsurface Flow Module and the Porous Media Flow Module — the mass source is applicable to the right-hand side of Equation 4-31 (where it is multiplied with the fracture thickness).

MASS SOURCE

Enter a value or expression for the Mass source $Q_{\rm m}$ (SI unit: kg/(m³·s)). The default is $0 \text{ kg/(m}^3 \cdot \text{s}).$

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

If you have the Subsurface Flow Module licensed, you can specify the pressure either directly or as an expression for the pressure head, H_p , or the hydraulic head, H; the hydraulic head and the pressure head relate to the pressure p as

$$H_p = \frac{p}{\rho g}; \quad H = H_p + D$$

where ρ is the fluid density (SI unit: kg/m³); g denotes the acceleration of gravity (SI unit: m/s^2); and *D* is the elevation (SI unit: m).

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa.

In case the Subsurface Flow Module is available, click the **Pressure head** button to enter a value or expression for H_p (SI unit: m). The default is 0 m. Click the **Hydraulic head** button to enter a value or expression for H (SI unit: m). The default is 0 m.

FRACTURE FLOW

For The Fracture Flow Interface, enter a value or expression for the Fracture thickness $d_{\rm f}$ (SI unit: m). The default is 0.1 m.



Flow in a Fractured Reservoir: Application Library path Subsurface Flow Module/Fluid Flow/fractured reservoir flow

Unsaturated Porous Medium

The **Unsaturated Porous Medium** node adds the Richards' equation (Equation 4-11) for flow in variably saturated porous media.

$$\rho \left(\frac{C_{\rm m}}{\rho g} + S_{\rm e} S_{\rm p} \right) \frac{\partial p}{\partial t} + \nabla \cdot \rho \left(-\frac{\kappa_{\rm r} \kappa}{\mu} (\nabla p + \rho g \nabla D) \right) = Q_{\rm m}$$
 (4-11)

The Unsaturated Porous Medium feature has two default subfeatures — the Fluid subfeature where the fluid density $\rho(SI \text{ unit: kg/m}^3)$ and viscosity μ (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m²)and porosity ε_{D} (dimensionless) are specified as well as the retention model.

COORDINATE SYSTEM SELECTION

Select a coordinate system from the **Coordinate system** list for the interpretation of directions in anisotropic material properties. The default is the Global coordinate system, and the list contains any additional orthonormal coordinate system (except boundary coordinate systems) added under the **Definitions** node.

The subnodes inherit these coordinate system settings. In particular, the **Permeability** or Hydraulic conductivity (in the Porous Matrix subnode) should be set according to the coordinate system selected in this section.

STORAGE MODEL

With this option, define the time storage term S_p in Equation 4-11.

- From density and porosity
- Linearized storage (default)
- User defined

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Gravity

The Gravity node is automatically added when Include gravity is selected at interface level in the Darcy's Law settings and it is active in all domains in which the Darcy's Law interface is applied.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

COORDINATE SYSTEM SELECTION

The Global coordinate system is selected by default. The Coordinate system list contains any additional coordinate systems that the model includes. It can be used when prescribing the direction of the gravitational forces.

GRAVITY

Specify either the acceleration vector or — in case you have a Subsurface Flow Module license — the elevation.

When Acceleration is selected from the list, enter the components of the Gravity vector g. The default value is g const which is the physical constant having the value 9.8066 m/s^2 .

- For 3D and 2D axisymmetric models, the default value is -g const in the z direction.
- For 2D models, the default value is -g const in the y direction.

When **Elevation** is selected from the list, specify the **Elevation** D (SI unit: m). Select the check box **Specify reference position** to define a reference elevation.

Select the acceleration of gravity from either the Darcy's Law interface Settings (default), or specify a user defined value. When the check box **Include gravity** is not selected in the Darcy's Law interface Settings, the elevation D is set equal to zero.

Cross Section

Use this node with 1D components to model domains with another cross-sectional area than the global one that is used in the interface **Physical Model** section. In 1D geometries, the pressure is assumed to be constant in the radial direction, and Darcy's Law accounts for that.

CROSS SECTION

Enter values for the **Cross-sectional area** A_c to set the cross section of the domain in the plane perpendicular to the 1D geometry.

Thickness

Use this node with 2D and 1D axisymmetric components to model domains with another thickness than the overall thickness that is specified in the interface Physical **Model** section. In 2D geometries, the pressure is assumed to be constant in the out-of-plane direction (z direction with default spatial coordinate names). In 1D axisymmetric geometries the thickness represents the z direction.

THICKNESS

Specify a value for the **Thickness** d_z of the domain in the out-of-plane direction. This value replaces the overall thickness in the domains that are selected in the Domain **Selection** section, and is used to multiply some terms into the heat equation.

Porous Electrode Coupling

Use the **Porous Electrode Coupling** node to define a mass source based on the volumetric current densities of one or multiple Porous Electrode Reaction nodes in an Electrochemistry interface.

The source (or sink) is proportional to the Molar mass (kg/mol) of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

SPECIES

Based on the number of species required for the model, use the **Add** (\bot) and **Delete**) buttons under the table to add or remove **Species**. Then enter a value for the Molar mass (kg/mol) in the applicable rows for each species.

The setting in the table will determine the number of available fields for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

Electrode Surface Coupling

Use the **Electrode Surface Coupling** node to define a combined wall and inflow/outflow boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flow is proportional to the Molar mass (kg/mol) of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

SPECIES

Based on the number of species required for the model, use the **Add** (+) and **Delete**) buttons under the table to add or remove **Species**. Then enter a value for the Molar mass (kg/mol) in the applicable rows for each species.

The setting in the table will determine the number of available field for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

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** $p_0(SI \text{ unit: Pa})$. Enter a relative pressure value in p_0 (SI unit: Pa).

For the Subsurface Flow Module, the **Pressure** node provides the pressure P_0 as a condition on edges in 3D models. Then select the edges under Edge Selection.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button (5) and select **Advanced** Physics Options in the Show More Options dialog box.

Pressure constraint on edges are available for use with the Fracture Flow boundary condition (which is available in the Subsurface Flow Module). This boundary condition needs constraints on the edges surrounding the fracture-flow boundary. In other cases, pressure constraints on edges are not implemented.

Mass Flux

Use the Mass Flux node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0 . A positive value of N_0 represents an inward mass flux whereas a negative value represents an outward mass flux. The units are based on the geometric entity: **Boundaries**: (SI unit: $kg/(m^2 \cdot s)$).

The Line Mass Source node adds mass flow originating from a tube of infinitely small radius.

SELECTION

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

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

LINE MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(m·s)). A positive value results in mass injection from the line into the computational domain, and a negative value means that the mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

Point Mass Source

The Point Mass Source node models mass flow originating from an infinitely small sphere centered around a point. It is available for points in 3D geometries.

POINT MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(s)). A positive value results in mass injection from the point into the computational domain, and a negative value means that the mass is removed from the computational domain.

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

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary. It has three options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity. A negative value represents an outflow velocity. The inlet velocity boundary condition is implemented as;

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = \rho U_0$$

where U_0 is a value or expression for the specified inward (or outward) Darcy velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas a negative value represents an outflow. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

PRESSURE

Use the **Pressure** option to specify the inlet pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example. Enter a value or expression for the **Pressure** $p_0(SI \text{ unit: Pa})$.

MASS FLOW

If you select ${f Mass flow}$ as the inlet condition, specify the total ${f Mass flow}$ rate $M_0({f SI}$ unit: kg/s), or the **Pointwise mass flux** $N_0(SI \text{ unit: kg/(m}^2 \cdot s))$.

With Mass flow rate boundary condition, positive values correspond to flow into the model domain:

$$-\int_{\partial\Omega} \rho(\mathbf{u} \cdot \mathbf{n}) \mathrm{d}S = M_0$$

where M_0 is a value or expression for the specified inward (or outward) Darcy flux.

Pointwise mass flux boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux.

CONSTRAINT SETTINGS

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

Symmetry

The **Symmetry** node describes a symmetry boundary. The following condition implements the symmetry condition on an axis or a flow divide:

$$\mathbf{n} \cdot \frac{\kappa}{\mu} \nabla p = 0$$

$$\mathbf{n} \cdot \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

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

No Flow

The **No Flow** node is the default boundary condition stating that there is no flow across impermeable boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

where $\bf n$ is the vector normal to the boundary. $\bf D$ is the elevation head which is set to zero for any other than Subsurface Flow Module applications.

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, **n** is the vector normal (perpendicular) to the interior boundary, ρ is the fluid density, \mathbf{u}_1 and \mathbf{u}_2 are the Darcy velocities in the adjacent domains (as defined in Equation 4-12) and N_0 is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{4-12}$$

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/(m²·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. It has different options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal outflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an outflow velocity whereas a negative value represents an inflow velocity.

$$-\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = \rho U_0$$

where U_0 is a specified value or expression for the outward (or inward) Darcy velocity.

PRESSURE

Similar to the inlet **Pressure** option, the outlet pressure on a boundary can be specified. Enter a value or expression for the **Pressure** $p_0(SI \text{ unit: Pa})$.

DISCHARGE

Enter a value or expression for the discharge Q_{D} to specify the volumetric flow rate through the boundary. The mass flux $\rho \mathbf{u}$ is related to the discharge as follows:

$$\int_{\partial\Omega} \rho \mathbf{u} \cdot \mathbf{ds} = \rho Q_D. \tag{4-13}$$

The mean normal outflow velocity at the boundary can then be calculated as U_{out} = $Q_{\rm D}/A$, where A is the cross sectional area of the boundary.

Note that this option is only available for Porous Media Flow and Subsurface Flow modules. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Precipitation

Enter a value or expression for the **Precipitation rate** which then contributes to the mass flux at the boundaries selected. If the boundary is inclined, a Slope correction can be applied.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Interior Wall

The Interior Wall boundary condition can only be applied on interior boundaries. It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of velocity and pressure across the boundary. The Interior Wall boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Thin Barrier

The **Thin Barrier** boundary condition models interior permeable walls, membranes, geotextiles, or perforated plates as thin permeable barriers. The Thin Barrier boundary condition can only be applied on interior boundaries.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

WALL

Enter a value or expression for the **Thickness** d_b (SI unit: m, the default is 0.1 m) and for the **Permeability** κ_b (SI unit: m²). The default **Permeability** κ_b uses the value **From** material. For User defined select Isotropic to define a scalar value or Diagonal, Symmetric, or Full to define a tensor value and enter another value or expression in the field or matrix.

Use the **Pressure Head** node to specify the pressure head (instead of the pressure) on a boundary. It adds this boundary condition for the pressure head $H_p = H_{p0}$, where H_{p0} is a known pressure head given as a number, a distribution, or an expression involving time, t, for example. The dimension of the pressure head is length (SI unit: m).

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

PRESSURE HEAD

Enter a value or expression for the **Pressure head** H_{p0} (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button (👼) and select **Advanced** Physics Options in the Show More Options dialog box.

Hydraulic Head

Use the **Hydraulic Head** node to specify the hydraulic head (instead of the pressure) on a boundary. This adds the Dirichlet condition for the hydraulic head $H = H_0$ where H_0 is a known hydraulic head given as a number, a distribution, or an expression involving time, t, for example.

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

HYDRAULIC HEAD

Enter a value or expression for the **Hydraulic head** H_0 (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

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

Atmosphere/Gauge

The Atmosphere/Gauge node specifies an atmospheric pressure or gauges the pressure to the atmospheric value. This means that the total hydraulic potential reduces to the gravitational pressure at the free surface. At a free surface, such as a spring or a seepage face, the pressure is atmospheric. If the pressures in the model is gauged to the

atmospheric value (p = 0), the total hydraulic potential reduces to the gravitational potential at the free surface — for example, the height of the free surface multiplied by the fluid weight, or $\rho_f gD$. This boundary condition sets the pressure at the boundary to zero and p = 0.

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

CONSTRAINT SETTINGS

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

Pervious Layer

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

The **Pervious Layer** node provides a boundary condition that describes a mass flux through a semi-pervious layer connected to an external fluid source at different pressure, pressure head, or hydraulic head. The model domain might connect to a larger body of water through the semi-pervious layer. This condition is represented with the following boundary condition:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = \rho R_{b} \left[\frac{(p_{b} - p)}{\rho g} + (D_{b} - D) \right]$$
 (4-14)

In this equation, p_b (SI unit: Pa) and D_b (SI unit: m) are the pressure and the elevation of the distant fluid source, respectively, and $R_{\rm h}$ (SI unit: 1/s) is the conductance of materials between the source and the model domain (conductance to flow in the semi-pervious layer adjacent to the boundary). Typically $R_b = K'/B'$, where K' is the hydraulic conductivity (SI unit: m/s) of the layer and B' (SI unit: m) is its thickness. Using logical relationships, it is possible to activate these expressions at different times or under various flow conditions.

When the pressure head H_D is specified instead of the pressure, the boundary condition is the following:

$$\mathbf{n} \cdot \rho K \nabla (H_p + D) = \rho R_{\rm b} [(H_{p \, \rm b} - H_p) + (D_{\rm b} - D)] \eqno(4-15)$$

 $H_{\rm pb}$ is the pressure head (SI unit: m) at the edge of the layer.

When the hydraulic head H is specified instead of the pressure head, the boundary condition becomes:

$$\mathbf{n} \cdot \rho K \nabla H = \rho R_{\mathbf{h}} [H_{\mathbf{h}} - H] \tag{4-16}$$

 $H_{\rm h}$ is the hydraulic head (SI unit: m) at the edge of the layer.

K in Equation 4-15 and Equation 4-16 is the hydraulic conductivity.

At a free surface, such as a water table or seepage face, the pressure is atmospheric (here taken to be zero), so the total hydraulic potential equals gravitational potential, which is defined on D.



Gravity effects are not active by default. Select the check box Include **gravity** to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

PERVIOUS LAYER

Specify the material properties whether to specify an external pressure, pressure head, or hydraulic head.

Select an External variable to specify — Pressure and elevation to specify the external pressure, Pressure head and elevation to specify the external pressure head, or Hydraulic head. For all selections, enter a value for the Conductance $R_{\rm b}$ (SI unit: 1/s).

- For Pressure and elevation enter an External pressure $p_{\mathbf{b}}$ (SI unit: Pa) and External elevation $D_{\mathbf{b}}$ (SI unit: m).
- For Pressure head and elevation enter an External pressure head H_{nb} (SI unit: m), H_{nb} (SI unit: m) and **External elevation** D_b (SI unit: m).
- For Hydraulic head enter the Hydraulic head H_{b} (SI unit: m).

Well

The **Well** feature is intended to model injection or production wells and is available with the Subsurface Flow Module.

WELL

Enter a value or expression for the **Well diameter** $d_{\rm w}$ (SI unit: m, the default is 0.1 m). Select the Well type from the list, Production or Injection well.

Specify either the Pressure (SI unit: Pa), Pressure head (SI unit: m), Hydraulic head (SI unit: m), or the Mass flow. If you select Mass flow, specify the total Mass flow rate (SI unit: kg/s), the Mass flow rate per unit length (SI unit: kg/(m·s)) or the Mass flux (SI unit: $kg/(m^2 \cdot s)$).

Fracture Flow

The Fracture Flow node adds fracture flow on boundaries using tangential derivatives to define the flow along interior boundaries representing fractures within a porous medium. It is implemented through The Fracture Flow Interface. Additional subnodes are available from the context menu (right-click the parent node) or from the Physics toolbar, Attributes menu.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Theory for the Richards' Equation Interface

The Richards' Equation Interface theory is described in this section:

- About Richards' Equation
- Retention and Permeability Relationships
- References for the Richards' Equation Interface

About Richards' Equation

Richards' equation models flow in variably saturated porous media. With variably saturated flow, hydraulic properties change as fluids move through the medium, filling some pores and draining others.

This discussion of the Richards' Equation interface begins with the propagation of a single liquid (oil or water). The pore space not filled with liquid contains an immobile fluid (air) at atmospheric pressure.

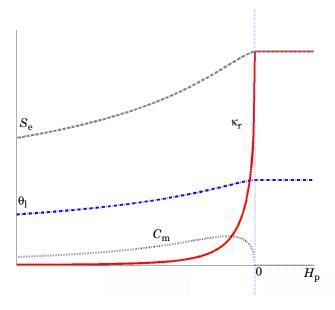


Figure 4-1: Fluid retention and permeability functions that vary with pressure head, as given by Van Genuchten formulas available in the Richards' Equation interface.

Many efforts to simplify and improve the modeling of flow in variably saturated media have produced a number of variants of Richards' equation since its appearance. The form that COMSOL Multiphysics solves is very general and allows for time-dependent changes in both saturated and unsaturated conditions (see Ref. 1 and Ref. 2):

$$\rho \left(\frac{C_{\rm m}}{\rho g} + S_{\rm e} S_{\rm p} \right) \frac{\partial p}{\partial t} + \nabla \cdot \rho \left(-\frac{\kappa_{\rm r} \kappa_{\rm s}}{\mu} (\nabla p + \rho g \nabla D) \right) = Q_{\rm m}$$
 (4-17)

where the pressure, p, is the dependent variable. In this equation, $C_{\rm m}$ represents the specific moisture capacity, $S_{\rm e}$ denotes the effective saturation, $S_{\rm p}$ is the storage coefficient, $\kappa_{\rm s}$ gives the hydraulic permeability at saturation, μ is the fluid dynamic viscosity, $\kappa_{\rm r}$ denotes the relative permeability, ρ is the fluid density, g is acceleration of gravity, D represents the elevation, and $Q_{\rm m}$ is the fluid source (positive) or sink (negative).

The fluid velocity across the faces of an infinitesimally small surface is

$$\mathbf{u} = -\frac{\kappa_{\rm r} \kappa_{\rm s}}{\mathfrak{u}} (\nabla p + \rho g \nabla D)$$

where \mathbf{u} is the velocity vector. The porous medium consists of pore space, fluids, and solids, but only the liquids move. The equation above describes the flux as distributed across a representative surface. To characterize the fluid velocity in the pores, COMSOL Multiphysics also divides \mathbf{u} by the liquid volume fraction, θ_1 . This interstitial, pore or average linear velocity is $\mathbf{u}_{a} = \mathbf{u}/\theta_{l}$.

Retention and Permeability Relationships

Richards' equation appears deceptively similar to the saturated flow equation set out in the Darcy's Law interface, but it is notoriously nonlinear (Ref. 3). Nonlinearities arise because the material and hydraulic properties θ_l, S_e, C_m , and κ_r vary for unsaturated conditions (for example, negative pressure) and reach a constant value at saturation (for example, pressure of zero or above). The volume of liquid per porous medium volume, θ_l , ranges from a small residual value θ_r to the total porosity ε_p . Its value is given in a constitutive relation in the model commonly defined as:

$$\theta_1 = \theta_r + S_e(\theta_s - \theta_r) \tag{4-18}$$

The variable θ_s is the saturated liquid volume fraction and therefore $\theta_s = \varepsilon_p$. The effective saturation, Se has a maximum value of 1 at saturation and usually follows a nonlinear relationship if the porous medium is unsaturated. The specific moisture capacity, $C_{\rm m}$, describes the change in $\theta_{\rm l}$ as the solution progresses, the slope on a plot of θ_l versus pressure (or pressure head). The relative permeability, κ_r , increases with moisture content and varies from a nominal value to 1 at saturation, which reveals that the fluid moves more readily when the porous medium is fully wet.

The Richards' Equation interface in COMSOL Multiphysics includes three retention models to define θ_l , S_e , C_m , and κ_r :

- The analytic formulas of van Genuchten.
- The analytic formulas of Brooks and Corey.
- User-defined expression.

The analytic formulas of van Genuchten (Ref. 4) and Brooks and Corey (Ref. 5) are so frequently used that they are synonymous with this variably saturated flow modeling. Posed in terms of pressure head $H_p = p/(\rho g)$, the analytic expressions require data for the saturated θ_s and residual θ_r liquid volume fractions as well as constants α , n, m, and l, which specify a particular medium type.

VAN GENUCHTEN

The van Genuchten equations define saturation when the fluid pressure is atmospheric (that is, $H_p = 0$). For unsaturated conditions ($H_p < 0$) the effective saturation is defined as:

$$S_{c} = \begin{cases} \frac{1}{1 + \left|\alpha H_{p}\right|^{nm}} & H_{p} < 0 \\ 1 & H_{p} \ge 0 \end{cases}$$

For the liquid volume fraction Equation 4-18 is used. The relative permeability is defined as

$$\kappa_{\rm r} = {\rm Se}^l \left[1 - \left(1 - {\rm Se}^{\frac{1}{m}} \right)^m \right]^2$$

which results in $\kappa_{\rm r}$ = 1 at saturation ($S_{\rm e}$ = 1). The specific moisture capacity is defined as:

$$C_{\rm m} = \frac{\alpha m}{1 - m} (\theta_{\rm s} - \theta_{\rm r}) Se^{\frac{1}{m}} \left(1 - Se^{\frac{1}{m}} \right)^m$$

here, the constitutive parameter m is equal to 1 - 1/n. The functions are highly nonlinear which is also depicted in Figure 4-2

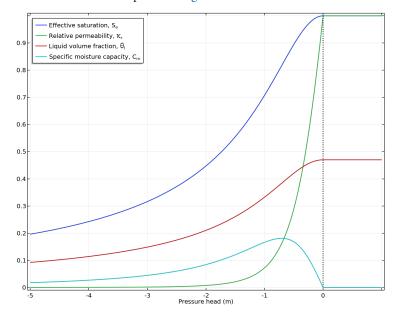


Figure 4-2: Van Genuchten retention functions for $\alpha = 1 \text{ m}^{-1}$, n = 2, and l = 0.5.

BROOKS AND COREY

With the Brooks and Corey approach, an air-entry pressure distinguishes saturated $(H_p\!>\!-1/\alpha)$ and unsaturated $(H_p\!<\!-1/\alpha)$ flow so that

$$Se = \begin{cases} \frac{1}{\left|\alpha H_{p}\right|^{n}} & H_{p} < -\frac{1}{\alpha} \\ 1 & -\frac{1}{\alpha} \le H_{p} \end{cases}$$

Again Equation 4-18 describes the liquid volume fraction. The relative permeability is defined as

$$\kappa_{\rm r} = Se^{\frac{\frac{2}{n} + l + 2}{}}$$

which results in $\kappa_{\rm r}$ = 1 at saturation ($S_{\rm e}$ = 1). The specific moisture capacity is defined as:

$$C_{\rm m} = \frac{-n}{H_p} (\theta_{\rm s} - \theta_{\rm r}) \frac{1}{S_{\rm e}}$$

Here, the constitutive parameter m is equal to 1 - 1/n. The functions are highly nonlinear which is also depicted in Figure 4-3

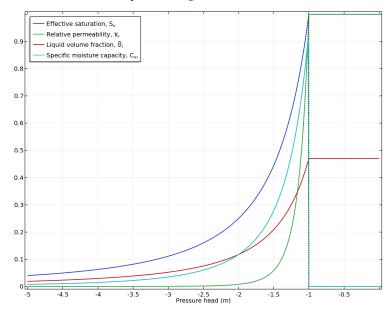


Figure 4-3: The Brooks and Corey retention functions for $\alpha = 1 \text{ m}^{-1}$, n = 2, and l = 0.5.

USER DEFINED

COMSOL Multiphysics also provides user-defined options for those who want to incorporate experimental data or arbitrary expressions to define these relationships. Enter expressions for θ_l , S_e , C_m , and κ_r directly.

References for the Richards' Equation Interface

- 1. J. Bear, Dynamics of Fluids in Porous Media, Elsevier Scientific Publishing, 1972.
- 2. J. Bear, Hydraulics of Groundwater, McGraw-Hill, 1979.
- 3. R.A. Freeze, "Three-dimensional, Transient, Saturated-unsaturated Flow in a Groundwater Basin," Water Resour. Res., vol. 7, no. 2, 1971.

- 4. M.Th. van Genuchten, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," Soil Sci. Soc. Am. J., vol. 44, 1980.
- 5. R.H. Brooks and A.T. Corey, "Properties of Porous Media Affecting Fluid Flow," J. Irrig. Drainage Div., ASCE Proc., vol. 72 (IR2), 1966.

The Richards' Equation Interface

The Richards' Equation (dl) interface (), found under the Porous Media and **Subsurface Flow** branch () when adding a physics interface, is used to analyze flow in variably saturated porous media. The analytic formulas of van Genuchten, Brooks, and Corey are available for modeling variably saturated flow, where hydraulic properties change as fluids move through the porous medium, filling some pores and draining others. 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** — **Richards' Equation: Unsaturated Porous Medium** (which adds the equation for the pressure and provides an interface for defining the fluid material and its properties, including the retention model), **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 Richards' Equation 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 d1.

PHYSICAL MODEL

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

GRAVITY EFFECTS

Gravity effects are active by default. Deselect the check box **Include gravity** to deactivate the acceleration of gravity.

Under Acceleration of gravity, enter the value for the acceleration of gravity (SI unit m/s²). The default value is taken from the predefined physical constant g const, which is the standard acceleration of gravity on earth.

DEPENDENT VARIABLES

The dependent variable (field variable) is for the **Pressure**. The name can be changed but the names of fields and dependent variables must be unique within a model.

DISCRETIZATION

You can choose the order of the shape functions used for the pressure variable solved by the Richards' Equation interface. The default shape functions are Quadratic Lagrange.

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



- Theory for the Richards' Equation Interface
- Domain, Boundary, Edge, Point, and Pair Nodes for the Richards' **Equation Interface**
- Physical Constants in the COMSOL Multiphysics Reference Manual



- Variably Saturated Flow: Application Library path Subsurface_Flow_Module/Fluid_Flow/variably_saturated_flow
- Pesticide Transport and Reaction in Soil: Application Library path Subsurface_Flow_Module/Solute_Transport/pesticide_transport

Domain, Boundary, Edge, Point, and Pair Nodes for the Richards' Equation Interface

The Richards' Equation Interface has the same domain, boundary, edge, point, and pair nodes described for the The Darcy's Law Interface.



Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface



In general, to add a node, go to the Physics toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the Attributes menu.





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



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

Flownet Plot

The Flownet plot is available for 2D and 2D axisymmetric models. This plot is created automatically when solving a model that includes a Richards' equation interface, and it is created by adding a Streamline plot for the velocity field and a contour plot for the pressure.

Theory for the Two-Phase Darcy's Law Interface

About the Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law interface combines Darcy's law (Equation 4-1) with the continuity equation (Equation 4-2) for the average density ρ . In the presence of two miscible fluid phases, the average density ρ and average viscosity μ depend on the composition of the mixture (Ref. 1). In the Two-Phase Darcy's Law interface these dependencies are given by

$$1 = s_1 + s_2 \tag{4-19}$$

$$\rho = s_1 \rho_1 + s_2 \rho_2 \tag{4-20}$$

$$\frac{1}{\mu} = s_1 \frac{\kappa_{r1}}{\mu_1} + s_2 \frac{\kappa_{r2}}{\mu_2} \tag{4-21}$$

Here, s_1 and s_2 represent the saturation of each phase, ρ_1 and ρ_2 the densities, and κ_{r1} and κ_{r2} the relative permeabilities. When either of the fluids is compressible, its density can be related to the pressure (for instance using the ideal gas law).

Beside the continuity equation for the mixture, the Two-Phase Darcy's Law interface also solves the transport equation for the fluid content of one of the phases, $c_1 = s_1 \rho_1$:

$$\frac{\partial}{\partial t} (\varepsilon_{\mathbf{p}} c_1) + \nabla \cdot (c_1 \mathbf{u}) = \nabla \cdot D_{\mathbf{c}} \nabla c_1 \tag{4-22}$$

Here, D_c (SI unit: m²/s) is the capillary diffusion coefficient, which can be directly specified or derived from a capillary pressure expression. Normally, the fluid content c_1 will be the concentration of the wetting phase.

When capillary pressure is selected as capillary model, the capillary diffusion coefficient is computed from the saturation of one of the phases and the capillary pressure:

$$D_{c} = \frac{\kappa_{r1}}{\mu_{1}} \kappa (s_{1} - 1) \frac{\partial p_{c}}{\partial s_{1}}$$
 (4-23)

The capillary pressure is defined as the pressure difference between the phases, and it can be defined as a function of saturation, $p_c(s_1)$.

Capillary Pressure Models

The capillary pressure can be a user defined expression, or it can be derived from van Genuchten (Ref. 2) or Brooks and Corey (Ref. 3) models.

For van Genuchten model, the expression for the capillary pressure as a function of saturation follows the curve

$$p_{c} = p_{ec} \left(\frac{1}{\frac{1}{s_{1}/m}} - 1 \right)^{1-m}$$
 (4-24)

where p_{ec} is the entry capillary pressure and m is a constitutive exponent.

For the Brooks and Corey model, the capillary pressure curve depends on saturation as

$$p_{c} = p_{ec} \frac{1}{s_{1}^{1/\lambda}} \tag{4-25}$$

where λ is the pore distribution index.

When capillary pressure is selected as capillary model, the relative permeabilities are also determined by the van Genuchten or Brooks and Corey models. For the van Genuchten model, the relative permeabilities are given by

$$\kappa_{\rm r1} = s_1^{l_{\rm vG}} (1 - (1 - s_1^{1/m_{\rm vG}})^{m_{\rm vG}})^2$$

$$\kappa_{\rm r2} = (1 - s_1)^{l_{\rm vG}} (1 - s_1^{1/m_{\rm vG}})^{2m_{\rm vG}}$$

where m_{vG} and l_{vG} are constitutive constants.

For the Brooks and Corey model, the relative permeabilities are given by

$$\kappa_{\rm r1}=s_1^{(3+2/\lambda)}$$

$$\kappa_{\rm r2} \, = \, (1 - s_1)^2 (1 - s_1^{(1 + 2/\lambda)})$$

where λ is again the pore distribution index.

References for the Two-Phase Darcy's Law Interface

- 1. Z. Chen, G. Huan, and Y. Ma, Computational Methods for Multiphase Flows in Porous Media. Philadelphia: Society for Industrial and Applied Mathematics, 2006.
- 2. M.Th. van Genuchten, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," Soil Sci. Soc. Am. J., vol. 44, 1980.
- 3. R.H. Brooks and A.T. Corey, "Properties of Porous Media Affecting Fluid Flow," J. Irrig. Drainage Div., ASCE Proc., vol. 72 (IR2), 1966.

The Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law (tpdl) interface (), found under the Porous Media and Subsurface Flow branch (No) when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It solves Darcy's law for the total pressure and the transport of the fluid content for one fluid phase. The physics interface can be used to model low velocity flows or media where the permeability and porosity are very small, for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. The physics interface can be used for stationary and time-dependent analyses.

The main feature is the Fluids and Matrix Properties node, which provides an interface for defining the two immiscible fluids properties along with the porous medium properties. The physics interface is available in 2D, 2D axisymmetric, and 3D.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — Fluids and Matrix Properties, No Flow (the default boundary condition), and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click Two-Phase **Darcy's Law** to select physics features from the context menu.

SETTINGS

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

The Name is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is tpd1.

PHYSICAL MODEL

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

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Pressure** and **Fluid content 1**. The name can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION

To display this section, click the **Show More Options** button () and select **Stabilization** from the **Show More Options** dialog box.

There are two consistent stabilization methods available — Streamline diffusion and Crosswind diffusion. Streamline diffusion is active by default. The Residual setting applies to both the consistent stabilization methods. Approximate residual is the default setting and it means that derivatives of the capillary diffusion tensor components are neglected. This setting is usually accurate enough and computationally faster. If required, select Full residual instead.

DISCRETIZATION

You can choose the order of the shape functions used for the pressure and fluid content variables solved by the Two-Phase Darcy's Law interface. The default shape functions are P2+P1 Lagrange.

To display all settings available in this section, click the **Show More Options** button (👼) and select Advanced Physics Options from the Show More Options dialog box.



- Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface
- Theory for the Two-Phase Darcy's Law Interface

Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law Interface has these domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), Physics context menu (Mac or Linux users), or right-click to access the context menu (all users).



In general, to add a node, go to the Physics toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid and Matrix Properties
- Inlet
- Initial Values
- Symmetry
- Interior Wall

- · Mass Flux
- No Flux
- Outlet
- Pressure and Saturation



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

Fluid and Matrix Properties

The Fluids and Matrix Properties node adds Equation 4-26 and Equation 4-27 and defines properties including density, dynamic viscosity, relative permeability, and porosity.

$$\frac{\partial}{\partial t}(\rho \varepsilon_p) + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{4-26}$$

$$\frac{\partial}{\partial t}(c_1 \varepsilon_p) + \nabla \cdot (c_1 \mathbf{u}) = \nabla \cdot D_c \nabla c_1 \tag{4-27}$$

CAPILLARY MODEL

The list defaults to Capillary diffusion or choose Capillary pressure.

For Capillary diffusion, choose Isotropic to define a scalar or Diagonal, Symmetric, or Full to enter a tensor, and then enter values or expressions in the D_c (SI unit: m^2/s) field or fields.

For Capillary pressure, select a Pressure model — van Genuchten (the default), Brooks and Corey, or User defined.

- For van Genuchten, enter an Entry capillary pressure p_{ec} (SI unit: Pa), the Constitutive relations constant m_{vG} (dimensionless), and Constitutive relations constant I_{vG} (dimensionless).
- For Brooks and Corey, enter an Entry capillary pressure p_{ec} (SI unit: Pa) and the Pore size distribution index λ_p (dimensionless).
- For User defined, enter a Capillary pressure p_c (SI unit: Pa).

FLUID I PROPERTIES

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

Define the properties for Fluid 1:

The default **Density** ρ_1 (SI unit: kg/m³) uses values **From material** based on the **Fluid I** selection. For **User defined** enter another value or expression. The default is 0 kg/m^3 .

Select a Dynamic viscosity μ_1 (SI unit: Pa·s). The default uses values From material as defined by the Fluid I selection. For User defined enter another value or expression. The default is 0 Pa·s.

Select the **Relative permeability** κ_{r1} (a dimensionless number between 0 and 1) for fluid 1. The default is 1.

FLUID 2 PROPERTIES

The settings to define the properties for Fluid 2 are similar as for Fluid 1.

MATRIX PROPERTIES

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

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From** material, defined by the Porous material selection. For User defined enter another value or expression The default is 0.

The default **Permeability** κ (SI unit: m^2) uses the value **From material**, as defined by the Porous material selection. For User defined select Isotropic to define a scalar or Diagonal, Symmetric or Full to enter a tensor and enter other values or expressions in the field or matrix.

Initial Values

The **Initial Values** node adds initial values for the pressure and the saturation of fluid 1 (that is, the fraction of that fluid inside the pore space) that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa. Enter a value or expression for the initial value of the **Saturation fluid I** s_1 (a dimensionless number between 0 and 1). The default value is 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

No Flux

The **No Flux** node is the default boundary condition stating that there is no flow across impervious boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \mathbf{u} = 0$$

where \mathbf{n} is the vector normal to the boundary.

Also, the No Flux boundary enforces a zero gradient condition for the fluid content across the selected boundary

$$\mathbf{n} \cdot \nabla c_1 = 0$$

Pressure and Saturation

Use the Pressure and Saturation node to specify the pressure and fluid volume fractions on a boundary. In many cases the distribution of pressure and saturation are known as numbers, distributions, or expressions involving time, t, for example.

PRESSURE AND SATURATION

Enter a value or expression for the **Pressure** p (SI unit: Pa), and for the **Saturation fluid I** s_1 (a dimensionless number between 0 and 1). The default values are 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

Mass Flux

Use the Mass Flux node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain

$$-\mathbf{n} \cdot \rho \mathbf{u} = N_0$$

where N_0 is a value or expression for the inward (or outward) Darcy's flux that is specified.

MASS FLUX AND SATURATION

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: kg/(m²·s)). A positive value of N_0 represents an inward mass flux, whereas a negative value represents an outward mass flux.

Enter a value or expression for the **Saturation fluid I** s_1 (a dimensionless number between 0 and 1) in the mass flux. The default value is 0.

Inlet

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot \rho \mathbf{u} = (s_1 \rho_1 + s_2 \rho_1) U_0$$

where U_0 is a specified value or expression for the inward (or outward) Darcy's velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas a negative value represents an outflow.

INLET

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity, whereas a negative value represents an outward velocity.

Enter a value or expression for the **Saturation fluid I** s_1 (a dimensionless number between 0 and 1). The default value is 0.

Outlet

The **Outlet** node adds a boundary condition for the outflow perpendicular (normal) to the boundary:

$$-\mathbf{n}\cdot D_c\nabla c_1 = 0$$

where D_c is the capillary diffusion (SI unit: m^2/s) and $c_1 = s_1 \rho_1$ is the fluid 1 content (SI unit: kg/m³). This means that the normal gradient of fluid saturation does not change through this boundary.

PRESSURE

Enter a value or expression for the **Pressure** p. The default value is 0. If the reference pressure p_{ref} , defined at the physics interface level is 0, enter the absolute pressure. Otherwise, enter the relative pressure.

Symmetry

The **Symmetry** node describes a symmetry boundary where there is no tangential flow. The following condition implements the symmetry condition on an axis or a flow divide:

$$-\mathbf{n} \cdot \rho \mathbf{u} = 0$$

$$-\mathbf{n} \cdot D_c \nabla c_1 = 0$$

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

Interior Wall

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

It is similar to the No Flux boundary available on exterior boundaries except that it applies on both sides of an internal boundary. It allows discontinuities of velocity and pressure across the boundary. The Interior Wall boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

Thin Barrier

The **Thin Barrier** boundary condition can only be applied on interior boundaries.

It is similar to the Interior Wall boundary available on interior boundaries except that it allows pressure and concentration gradients across the boundary. The Thin Barrier boundary condition can be used to avoid meshing thin permeable structures by applying flux condition on interior curves and surfaces instead.

Theory for the Fracture Flow Interface

The Fracture Flow Interface theory is described in this section:

- About Fracture Flow
- Equations and Inputs

About Fracture Flow

The Fracture Flow interface uses tangential derivatives to define the flow along the interior boundaries representing fractures within a porous (or solid) block. Use this physics interface on boundaries in 3D, 2D, and axisymmetric geometries.



Fracture Flow is also available as a boundary condition in the Darcy's Law and Richards' Equation interfaces.

The physics interface uses the tangential version of Darcy's law:

$$\mathbf{q}_{\mathbf{f}} = -\frac{\kappa_{\mathbf{f}}}{\mu} d_{\mathbf{f}} (\nabla_{\mathbf{T}} p + \rho g \nabla_{\mathbf{T}} D) \tag{4-28}$$

Here, \mathbf{q}_f is the volume flow rate per unit length in the fracture, κ_f is the fracture's permeability, μ is the fluid dynamic viscosity, d_f is the aperture or fracture thickness, $\nabla_{\rm T}$ denotes the gradient operator restricted to the fracture's tangential plane, p is the pressure, ρ is the fluid density, g is the acceleration of gravity, and D represents the vertical coordinate.



Gravity effects are not active by default. Select the check box Include **gravity** to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

The variable \mathbf{q}_f gives the volume flow rate per unit length of the fracture. The mean fluid velocity within the fracture is $\mathbf{u}_{\rm f} = \mathbf{q}_{\rm f}/d_{\rm f}$.

It is also possible to use the hydraulic conductivity of the fracture, K_f (SI unit: m/s), to define the capacity to transmit flow instead of using the fracture's permeability $\kappa_{\rm f}$ and fluid viscosity μ . These quantities are related by

$$\frac{\kappa_{\rm f}}{\mu} = \frac{K_{\rm f}}{\rho g}$$

The hydraulic conductivity represents properties of both fluid and porous matrix. If the model is defined using the hydraulic conductivity, Equation 4-28 changes to

$$\mathbf{q}_{\mathrm{f}} = -\frac{K_{\mathrm{f}}}{\rho g} d_{\mathrm{f}} (\nabla_{\mathrm{T}} p + \rho \, g \nabla_{\mathrm{T}} D) \tag{4-29}$$

The Cubic law equation describes the permeability of the fracture from the aperture or fracture's thickness d_f and the roughness factor f_f

$$\kappa_{\rm f} = \frac{d_{\rm f}^2}{12f_{\rm f}}$$

If the model is defined using the Cubic law equation, the expression for flow rate per unit length in the fracture in Equation 4-28 changes to

$$\mathbf{q}_{\mathrm{f}} = -\frac{d_{\mathrm{f}}^{3}}{12\mu f_{\mathrm{f}}} (\nabla_{\mathrm{T}} p + \rho g \nabla_{\mathrm{T}} D) \tag{4-30}$$

Together with the material properties, Equation 4-28 above, in combination with the continuity equation integrated over the fracture cross section, produces a single equation for the pressure.

$$d_{\rm f} \frac{\partial}{\partial t} (\varepsilon_{\rm f} \rho) + \nabla_T \cdot (\rho \mathbf{q}_{\rm f}) = d_{\rm f} Q_{\rm m} \tag{4-31}$$

where ε_f is the fracture porosity, and Q_m is the mass source term (SI unit: kg/(m³·s)). The aperture or fracture thickness d_f can vary along the fracture and therefore appears on both sides of the equation.

The physics interface solves for the same dependent variable as for the equation in the porous medium, the pressure p.

Equations and Inputs

Two material models are supported: Fluid and Fracture Properties and the Storage Model.

FLUID AND FRACTURE PROPERTIES

This is the default setting of the Fracture Flow interface, and implements the fracture flow as described in Equation 4-31. The values for the fluid properties (density and dynamic viscosity) can be taken from the material node or be defined by an arbitrary expression. The same can be done for the fracture's properties, such as porosity and permeability. Enter the fracture's thickness in the corresponding field.

STORAGE MODEL

The governing equation takes the slightly different form, compared to Equation 4-31:

$$\rho S_{\mathbf{f}} d_{\mathbf{f}} \frac{\partial p}{\partial t} - \nabla_T \cdot (\rho \mathbf{q}_{\mathbf{f}}) = d_{\mathbf{f}} Q_m$$

where $S_{\mathbf{f}}$ is the fracture storage coefficient (SI unit: 1/Pa).

In contrast to the Darcy's Law and Richards' Equation interfaces, the storage coefficient is always a user-defined expression in the Fracture Flow interface.

The Fracture Flow Interface

The Fracture Flow (esff) interface (), found under the Porous Media and Subsurface Flow branch () when adding a physics interface, is used to simulate flow along interior boundaries representing fractures within a porous or solid medium. The physics interface uses a variant of Darcy's law and 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 — Fluid and Fracture Properties, No Flow (the default boundary condition), and **Initial Values.** Then, from the **Physics** toolbar, add other nodes that implement, for example, mass sources and conditions on edges or points. You can also right-click **Fracture 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 esff.

PHYSICAL MODEL

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

GRAVITY EFFECTS

Gravity effects are not active by default. Select the check box **Include gravity** to activate the acceleration of gravity.

Under **Acceleration of gravity** enter the value for the acceleration of gravity g (SI unit: m/s^2). The default value is the predefined constant $g_const.$

DISCRETIZATION

You can choose the order of the shape functions used for the pressure variable solved by the Fracture Flow interface. The default shape functions are **Quadratic** Lagrange.

DEPENDENT VARIABLES

The dependent variable (field variable) is for the **Pressure**. The name can be changed but the names of fields and dependent variables must be unique within a model.

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



- Domain, Boundary, Edge, Point, and Pair Nodes for the Fracture Flow Interface
- Theory for the Fracture Flow Interface
- Physical Constants in the COMSOL Multiphysics Reference Manual

Domain, Boundary, Edge, Point, and Pair Nodes for the Fracture Flow Interface

The Fracture Flow Interface has the 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.

DOMAIN

- Fluid and Fracture Properties
- Aperture
- · Initial Values
- Mass Source
- Storage Model
- Gravity
- Thickness



Storage Model and Mass Source are described for the Darcy's Law interface and are applied to boundaries instead of domains.

BOUNDARY CONDITIONS

The boundary conditions for this physics interface are similar to the boundary conditions for The Darcy's Law Interface but are applied to edges in 3D and points in 2D. Edges and points form the "boundaries" of the geometries where the Fracture Flow interface is defined, which are faces in 3D and boundaries in 2D.





In the descriptions for these nodes, replace the **Boundary Selection** section with the Edge Selection (3D) or Point Selection (2D) section when using the Fracture Flow interface.

The following nodes are available on exterior boundaries (edges and points) and described for The Darcy's Law Interface:

- Pressure
- Pressure Head
- Hydraulic Head
- Inlet
- Outlet

- · Mass Flux
- Symmetry
- No Flow (the default)
- Atmosphere/Gauge
- · Pervious Layer

Note that some of the boundary conditions mentioned above are only available for certain modules. For detailed information, see

https://www.comsol.com/products/specifications/.

The relevant physics interface condition at interior edges is continuity. In addition, the following edge conditions are available on interior edges:

- Pressure
- Pervious Layer



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

Fluid and Fracture Properties

The **Fluid and Fracture Properties** node adds Equation 4-2 (excluding any mass sources) on the selected boundary for the pressure and provides an interface for defining the fluid material and its properties, including the effective porosity.



All the nodes are the same as with the Darcy's Law interface except where indicated.

FLUID PROPERTIES

The default Fluid material uses the Domain material (the material defined for the domain). Select another material as needed.

The default Density ρ (SI unit: kg/m³) uses values From material based on Fluid material selected. For User defined enter another value or expression. The default is 0 kg/m^3 .

The default **Dynamic viscosity** μ (SI unit: Pa·s) uses values **From material** based on the Fluid material selected. For User defined enter another value or expression. The default is 0 Pa·s.



If Hydraulic conductivity is selected as the Permeability model (see the Matrix Properties section), dynamic viscosity is not available. The hydraulic conductivity is defined using a combination of fluid and matrix properties and replaces the need of defining the dynamic viscosity.

FRACTURE PROPERTIES

The default Porous material uses the Boundary material (the material defined for the fracture domain) for the fracture. Select another material as needed.

Porosity

The default **Porosity** in the fracture ε_f (a dimensionless number between 0 and 1) uses values From material based on the Porous material selected. For User defined enter another value or expression. The default is 0.

Permeability Model

Select a **Permeability model** to specify the capacity of the porous material to transmit flow: Permeability to define the permeability of the fracture, Hydraulic conductivity,

which is a combination of permeability and the dynamic viscosity of water, or **Cubic law** to define the permeability as a function of the fracture's aperture.

- For **Permeability** $\kappa_f(SI \text{ unit: } m^2)$ the default uses values **From material** as defined by the Porous material selected. For User defined select Isotropic to define a scalar value or Diagonal, Symmetric, or Full to enter a tensor value.
- For **Hydraulic conductivity** K (SI unit: m/s) enter a value or expression and select Isotropic to define a scalar value or Diagonal, Symmetric, or Full to enter a tensor value.
- For Cubic law enter a value or expression for the Roughness factor $f_{\rm f}$.

Storage Model

The settings are the same as for the Fluid and Fracture Properties. Enter a value or expression for Storage S (SI unit: 1/Pa).

Aperture

The default node to specify the fracture's aperture. Enter a value or expression for the **Aperture** d_f (SI unit: m). The default is 1 mm.

Initial Values

The **Initial Values** node adds an initial value for the pressure, pressure head, or hydraulic head pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

- Select the **Pressure** (the default) button to enter a value or expression for the initial value of the pressure p (SI unit: Pa). The default is 0 Pa.
- Select Pressure head to enter a value or expression for $H_{\mathbf{p}}$ (SI unit: m).
- Select **Hydraulic head** to enter a value or expression for H (SI unit: m).

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 fast-moving fluids in porous media with the kinetic potential from fluid velocity, pressure, and gravity to drive the flow. These equations extend Darcy's law to describe the dissipation of the kinetic energy by viscous shear as with the Navier-Stokes equations. Consequently, this physics interface well suits transitions between slow flow in porous media governed by Darcy's law and fast flow in channels described by the Navier-Stokes equations. Interesting uses of a Brinkman and Navier-Stokes coupling include modeling of the hyporheic zone near a river, the flow of oil through a reservoir to a well perforation, and non-Newtonian flows.

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:

$$\frac{\partial}{\partial t}(\varepsilon_{\rm p}\rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m} \tag{4-32}$$

$$\frac{\rho}{\varepsilon_{p}} \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon_{p}} \right) =
-\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_{p}} \left\{ \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} \right] - \left(\kappa^{-1} \mu + \frac{Q_{m}}{\varepsilon_{p}^{2}} \right) \mathbf{u} + \mathbf{F}$$
(4-33)

In these equations:

- μ (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- **u** (SI unit: m/s) is the velocity vector
- ρ (SI unit: kg/m³) is the density of the fluid
- p (SI unit: Pa) is the pressure
- $\varepsilon_{\rm p}$ is the porosity
- κ (SI unit: m^2) is the permeability of the porous medium, and
- $Q_{\rm m}$ (SI unit: kg/(m³·s)) is a mass source or sink

Influence of gravity and other volume forces can be accounted for via the force term **F** (SI unit: $kg/(m^2 \cdot s^2)$).

When the Neglect inertial term (Stokes flow) check box is selected, the term $(\mathbf{u} \cdot \nabla)(\mathbf{u}/\varepsilon_{\mathbf{p}})$ on the left-hand side of Equation 4-33 is disabled.

The mass source, $Q_{\rm m}$, accounts for mass deposit and mass creation within the domains. The mass exchange is assumed to occur at zero velocity.

The Forchheimer and Ergun drag options add a viscous force proportional to the square of the fluid velocity, $\mathbf{F} = -\rho \beta |\mathbf{u}|\mathbf{u}$, on the right-hand side of Equation 4-33; see References for the Darcy's Law Interface for details.

In case of a flow with variable density, Equation 4-32 and Equation 4-33 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

$$\frac{\partial}{\partial t}(\varepsilon_{\mathbf{p}}\rho) + \mathbf{u} \cdot \nabla \rho = 0$$

and the continuity equation (Equation 4-32) reduces to

$$\rho \nabla \cdot \mathbf{u} = Q_{\rm m}$$

References for the Brinkman Equations Interface

- 1. D. Nield and A. Bejan, Convection in Porous Media, 3rd ed., Springer, 2006.
- 2. M. Le Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," J. Fluid Mech., vol. 550, pp. 149-173, 2006.

The Brinkman Equations Interface

The Brinkman Equations (br) interface (), found under the Porous Media and Subsurface Flow branch (🔊) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. The physics interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. To simplify the equations, select the Stokes–Brinkman flow feature to reduce the dependence on inertial effects when the Reynolds number is significantly less than 1. The physics interface can be used for stationary and time-dependent analyses.

The main node is the Porous Medium feature, which adds the Brinkman equations and provides interfaces for defining the fluid material and the porous matrix.

When this physics interface is added, the following default nodes are also added in the Model Builder — Porous Medium, Wall (the default boundary type, using No slip as the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Brinkman Equations** to select physics features from the context menu.

The boundary conditions are essentially the same as for the Laminar Flow interface. Differences exist for the following boundary types: Outlet, Symmetry, Open Boundary, and Boundary Stress where the viscous part of the stress is divided by the porosity to appear as

$$\frac{1}{\varepsilon_{p}} \left\{ \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right\}$$

In the COMSOL Multiphysics Reference Manual see Table 2-4 for links to common sections such as Discretization, Consistent Stabilization, and Inconsistent Stabilization, and **Advanced Settings** sections, all accessed by clicking the **Show** button (**5**) and choosing the applicable option. You can also search for information: press F1 to open the Help window or Ctrl+F1 to open the **Documentation** window.

SETTINGS

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

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>. <variable name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

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

PHYSICAL MODEL

This node specifies the properties of the Brinkman Equations interface, which describe the overall type of fluid flow model.

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Brinkman equations to model constant density flow. Alternatively, from the Compressibility list select Weakly compressible flow which should be used when the pressure dependency of the density can be neglected, or Compressible flow (Ma<0.3) to solve for the full compressible flow of which, however, the Mach number must be below 0.3.

Swirl Flow

For 2D axisymmetric models, select the Swirl flow check box to include the swirl velocity component, that is the velocity component u_{σ} in the azimuthal direction. While u_{α} can be nonzero, there can be no gradients in the φ direction.

Note that this feature is only available for specific modules. See https://www.comsol.com/products/specifications/ for a detailed overview.

Neglect Inertial Term (Stokes-Brinkman Flow)

The Neglect inertial term (Stokes-Brinkman) check box is selected by default to model flow at low Reynolds numbers for which the inertial term can be neglected. This results in the linear Stokes-Brinkman equations.

Include Gravity

Gravity is not included by default. Select the **Include gravity** check box to activate the acceleration of gravity. This automatically adds a global Gravity feature node to the interface model tree, and the buoyancy force is included in the Equations.

Also, when the Include gravity check box is selected, the Use reduced pressure option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Porous Treatment of No Slip Condition

Choose how the No Slip condition on Wall boundaries and Interior Wall boundaries adjacent to Porous Medium should be treated. The options are Standard no slip formulation (default) and Porous slip. The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in the The Laminar Flow and Creeping Flow Interfaces section.

Reference Pressure Level

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

Reference Temperature Level

Enter a Reference temperature level $T_{\rm ref}({\rm SI~unit};{\rm K})$. The default value is 293.15[K].

Reference Position

If Include gravity is selected, a Reference position $r_{ref}(SI \text{ unit: m})$ can be specified which is then used for the calculation of the hydrostatic pressure.

TURBULENCE

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS** (Reynolds-Averaged Navier–Stokes). If turbulent flow is activated, one of the following Turbulence models can be chosen: Algebraic yPlus, L-VEL, and k- ε , and Wall functions are preset for Wall treatment. For more information about turbulence modeling, see Theory for the Turbulent Flow Interfaces in the CFD Module User's Guide.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field u** (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

ADVANCED SETTINGS

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

The Use pseudo time stepping for stationary equation form option adds pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. When selected, a **CFL number expression** should also be defined. For

the default Automatic option, the local CFL number (from the Courant-Friedrichs-Lewy condition) is determined by a PID regulator.

> • Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface



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- 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



Free Convection in a Porous Medium: Application Library path Subsurface_Flow_Module/Heat_Transfer/convection_porous_medium

Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface

The Brinkman Equations Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



In general, to add a node, go to the Physics toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

These nodes are described in this section:

- · Porous Medium
- · Initial Values
- · Mass Source

- Volume Force
- Fluid Properties

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

- Flow Continuity
- Inlet
- Line Mass Source
- · Boundary Stress
- Outlet
- Open Boundary

- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Wall



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

Porous Medium

The **Porous Medium** node adds the Brinkman equations: Equation 4-25 and Equation 4-26 (excluding any mass sources). It has two default subfeatures — the Fluid subfeature where the fluid density $\rho(SI \text{ unit: kg/m}^3)$ and dynamic viscosity $\mu(SI \text{ viscosity})$ unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit: $\text{m}^2)$ and porosity ϵ_p (dimensionless) are specified.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- Darcian flow (default) defines a linear relationship.
- Non-Darcian flow defines a nonlinear relationship due to turbulence or inertial effects.

Fluid

This node defines the material properties of the fluid of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

Specify the **Density** ρ and the **Dynamic viscosity** μ (SI unit: Pa·s) of the fluid. The defaults use values From material, for User defined enter a value or expression.

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

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The **Porosity** $\varepsilon_{\rm p}$ (a dimensionless number between 0 and 1) uses by default the value From material. For User defined the default value is 1.

Select a Permeability model to specify the capacity of the porous material to transmit flow. Depending on the Flow model selection in the parent Porous Medium feature node you can choose between the following options:

- **Permeability** (the default) to directly enter the permeability of the porous matrix or Kozeny-Carman to define the permeability from the porosity and mean Particle diameter for Darcian flow or
- Forchheimer or Ergun for Non-Darcian flow.

Note that some of these options are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

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

For Kozeny-Carman, enter the mean Particle diameter $d_{\rm p}$ (SI unit: m), the default value is 0.5 mm.

In case a Non-Darcian flow model is chosen in the parent node, Forchheimer is the default selection for the Permeability model. For Forchheimer, the default Permeability $\kappa(SI \text{ unit: m}^2)$ uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_E can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** $d_{\rm p}$ (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow* Module User's Guide.



- About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide
- Permeability Models in the Porous Media Flow Module User's Guide

Mass Source

The Mass Source node adds a mass source (or mass sink) Q_{m} to the right-hand side of the continuity equation: Equation 4-32. 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.

$$\frac{\partial}{\partial t}(\varepsilon_{\rm p}\rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m} \tag{4-34}$$

DOMAIN SELECTION

Only Porous Matrix domains are available.

MASS SOURCE

Enter a value or expression for the **Source term** $Q_{\rm br}$ (SI unit: kg/(m³·s)). The default is $0 \text{ kg/(m}^3 \cdot \text{s})$.

Use the **Volume Force** node to specify the force \mathbf{F} on the right-hand side of Equation 4-33. It then acts on each fluid element in the specified domains.

$$\begin{split} & \frac{\rho}{\varepsilon_{\mathrm{p}}} \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon_{\mathrm{p}}} \right) = \\ & - \nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_{\mathrm{p}}} \left\{ \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} \right] - \left(\kappa^{-1} \mu + \frac{Q_{\mathrm{m}}}{\varepsilon_{\mathrm{p}}^{2}} \right) \mathbf{u} + \mathbf{F} \end{split}$$

$$(4-35)$$

VOLUME FORCE

Enter the components of **Volume force 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 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 nonporous domains. The node also provides an interface for defining the material properties of the fluid.

MODEL INPUTS

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

Temperature

By default, the single-phase flow interfaces are set to model isothermal flow. Hence, the Temperature is User defined and defaults to 293.15 K. If a Heat Transfer interface is included in the component, the temperature may alternatively be selected from this physics interface. All physics interfaces have their own tags (Name). For example, if a

Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

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

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

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

FLUID PROPERTIES

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible.

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

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the Physical Model settings. It defines the gravity forces from the **Acceleration of gravity** value. When a turbulence model that solves for the turbulent

kinetic energy, k, is used, the option Include buoyancy-induced turbulence is available. When selected, the Buoyancy contribution is by default set to Automatic from multiphysics. Contributions are only obtained from multiphysics couplings that support buoyancy-induced turbulence, such as Nonisothermal Flow. If the Buoyancy contribution is switched to User defined, a text field for the Turbulent Schmidt number appears. See also Theory for Buoyancy-Induced Turbulence in the CFD Module User's Guide.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

ACCELERATION OF GRAVITY

The Acceleration of gravity (SI unit m/s, default value $-g_{const}\mathbf{e_z}$ in 2D axial symmetry and 3D and $-g_{const}\mathbf{e_v}$ in 2D) is used to define the gravity forces. It should be a global quantity.

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, **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.

The Free and Porous Media Flow Interface

The Free and Porous Media Flow (fp) interface () is found under the Porous Media and Subsurface Flow branch () when adding a physics interface. It is used to compute fluid velocity and pressure fields of single-phase flow where free flow is connected to porous media. The Free and Porous Media Flow interface is used over at least two different domains: a free channel and a porous medium. The physics interface is well suited for transitions between slow flow in porous media, governed by the Brinkman equations, and fast flow in channels described by the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. The physics interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the Model Builder — Fluid Properties, Wall, and Initial Values. Then, from the Physics toolbar, add a **Porous Medium** node to be used on the domain selection corresponding to the porous media, or add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click Free and Porous Media Flow to select physics features from the context menu.

SETTINGS

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

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

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

PHYSICAL MODEL

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Navier– Stokes and Brinkman equations to model constant density flow. If required, select Weakly compressible flow from the Compressibility list, to account for small variations in

the density, which are only dependent on the temperature (nonisothermal flow) or Compressible flow (Ma<0.3) for fully compressible flow. However, for the flow modeled with this physics interface, the Mach number must be below 0.3.

Swirl Flow

For 2D axisymmetric components, select the **Swirl flow** check box to include the swirl velocity component, that is the velocity component u_{ω} in the azimuthal direction. While u_{α} can be nonzero, there can be no gradients in the φ direction. Note that this feature is only available for specific modules. Visit

https://www.comsol.com/products/specifications/ for a detailed overview.

Neglect Inertial Term

Select the Neglect inertial term (Stokes flow) check box if the inertial forces are small compared to the viscous forces.

Enable porous media domains

The **Enable porous media domains** check box is selected by default to solve the Brinkman equations in porous domains. If it is unchecked, the **Porous Medium** node is no longer available in this interface.

Include Gravity

Gravity is not included by default. Select the **Include gravity** check box to activate the acceleration of gravity. This automatically adds a global Gravity feature node to the interface model tree, and the buoyancy force is included in the Equations.

Also, when the Include gravity check box is selected, the Use reduced pressure option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Porous Treatment of No Slip Condition

Choose how the **No Slip** condition on internal boundaries should be treated. The options are Standard no slip formulation (default) and Porous slip. The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in the The Laminar Flow and Creeping Flow Interfaces section.

Reference Pressure Level

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

Reference Temperature

Enter a Reference temperature T_{ref} (SI unit: K). The default value is 293.15[K].

Reference Position

If Include gravity is selected, a Reference position $r_{\rm ref}({\rm SI~unit:m})$ can be specified which is then used for the calculation of the hydrostatic pressure.

TURBULENCE

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS** (Reynolds-Averaged Navier–Stokes) or Large Eddy Simulation (which is only available in 3D). If turbulent flow is activated, you can choose from different Turbulence models and options for **Wall treatment**. For a description of the different turbulence models, wall treatment options, and turbulence model parameters see Theory for the Turbulent Flow Interfaces in the CFD Module User's Guide.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field 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



Forchheimer Flow: Application Library path Subsurface_Flow_Module/Fluid_Flow/forchheimer_flow

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
- Gravity
- Initial Values

- · Porous Medium
- · Mass Source
- Volume Force
- Wall

Note that some features are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/).

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

- No Viscous Stress
- Flow Continuity
- Inlet
- Line Mass Source
- Outlet

- Open Boundary
- · Periodic Flow Condition
- · Point Mass Source
- Pressure Point Constraint
- Symmetry



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

Fluid Properties

Use the Fluid Properties node to define the fluid material, density, and dynamic viscosity.

FLUID PROPERTIES

The default Fluid material uses the Domain material (the material defined for the domain). Select another material as needed.

The default **Density** ρ (SI unit: kg/m³) uses values **From material** based on the **Fluid** material selection. For User defined enter another value or expression. The default is 0 kg/m^3 .

The Dynamic viscosity μ (SI unit: Pa·s) uses values From material based on the Fluid material selection. For User defined enter another value or expression. The default is 0 Pa·s.

Porous Medium

The **Porous Medium** node adds the Brinkman equations (excluding any mass sources) to the interface. It has two default subfeatures — the Fluid subfeature where the fluid density $\rho(SI \text{ unit: kg/m}^3)$ and dynamic viscosity $\mu(SI \text{ unit: Pa·s})$ are defined and the Porous Matrix subfeature where the permeability κ (SI unit: m²) and porosity $\varepsilon_{\rm p}$ (dimensionless) are specified.

FLOW MODEL

Define if the flow follows a linear or nonlinear pressure-velocity relationship.

- Darcian flow (default) defines a linear relationship.
- Non-Darcian flow defines a nonlinear relationship due to turbulence or inertial effects.

Fluid

This node defines the material properties of the fluid of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

FLUID PROPERTIES

Specify the **Density** ρ and the **Dynamic viscosity** μ (SI unit: Pa·s) of the fluid. The defaults use values From material, for User defined enter a value or expression.

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

Porous Matrix

This node defines the porosity and material properties of the solid matrix of the Porous Medium parent node.

MODEL INPUT

This section contains fields and values that are inputs for expressions defining material properties. If such user-defined property groups are added, the model inputs appear here.

MATRIX PROPERTIES

The **Porosity** \mathcal{E}_p (a dimensionless number between 0 and 1) uses by default the value From material. For User defined the default value is 1 which is equivalent to free flow.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Depending on the Flow model selection in the parent Porous Medium feature node you can choose between the following options:

- Permeability (the default) to directly enter the permeability of the porous matrix or Kozeny-Carman to define the permeability from the porosity and mean Particle diameter for Darcian flow or
- Forchheimer or Ergun for Non-Darcian flow.

Note that some of these options are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

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

For Kozeny-Carman, enter the mean Particle diameter $d_{\rm p}$ (SI unit: m), the default value is 0.5 mm.

In case a Non-Darcian flow model is chosen in the parent node, Forchheimer is the default selection for the Permeability model. For Forchheimer, the default Permeability $\kappa(SI \text{ unit: } m^2)$ uses the value **From material**. Furthermore, the dimensionless **Forchheimer parameter** c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** $d_{\rm p}$ (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow* Module User's Guide.



- About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide
- Permeability Models in the Porous Media Flow Module User's Guide

Mass Source

Enter a value or expression for an optional mass source (or sink) Source term Q_{m} (SI unit: kg/(m³·s)). This term accounts for mass deposit or mass creation within porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

Volume Force

The **Volume Force** node specifies the force \mathbf{F} on the right-hand side of the Navier– Stokes or Brinkman equations, depending on whether a Fluid Properties or Porous Medium node is active on the domain. It then acts on each fluid element in the specified domains.

VOLUME FORCE

Enter the components of the **Volume force 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 u (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Gravity

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

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

ACCELERATION OF GRAVITY

The Acceleration of gravity (SI unit m/s, default value $-g_{const}e_z$ in 2D axial symmetry and 3D and $-g_{const}e_{y}$ in 2D) is used to define the gravity forces. It should be a global quantity.

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 Slip¹

· Leaking Wall

Slip

No Slib

No slip is the default boundary condition for a stationary solid wall for laminar flow (and SST, Low Re k-ɛ, Algebraic yPlus, L-VEL, and Spalart-Allmaras turbulence models). The condition prescribes $\mathbf{u} = 0$; that is, the fluid at the wall is not moving.

Slip

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

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_1$ through a perforated wall. The components of the **Fluid velocity \mathbf{u}_l** on the leaking wall should be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button (50) and selecting **Advanced Physics Options.**



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

Shallow Water Equations Interface

The physics interface described in this chapter is found under the **Fluid** Flow>Shallow Water Equations branch (\blacksquare).

In this chapter:

- The Shallow Water Equations, Time Explicit Interface
- Theory for the Shallow Water Equations Interface.

The Shallow Water Equations, Time Explicit Interface

In this section:

- The Shallow Water Equations, Time Explicit Interface
- Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface



Theory for the Shallow Water Equations Interface

The Shallow Water Equations, Time Explicit Interface

The Shallow Water Equations, Time Explicit (swe) interface (), found under the **Shallow Water Equations** branch () when adding a physics interface, is used to solve the Shallow Water equations in a 1D or 2D geometry. These equations model the flow of a free surface in a fluid under the assumption that the horizontal scale is much greater than the vertical length scale. They are frequently used for modeling both oceanographic and atmospheric fluid flow. Models of such systems can be used to predict areas affected by pollution, coastal erosion, and polar ice-cap melting, provided the fluid layer is shallow enough.

Comprehensive modeling of such phenomena using physical descriptions such as the Navier-Stokes equations can often be problematic, due to the scale of the modeling domains as well as the resolution of free surfaces. The shallow water equations, of which there are a number of representations, provide an easier description of such phenomena.

A typical configuration for the flow of fluid in a shallow layer is shown in Figure 5-1. This physics interface approximates free surface problems where the thickness h of the fluid layer, or water depth, is small compared to the lateral dimensions of the geometry. The lower boundary of the fluid is treated as a nonpenetrable wall and has a height $h_h(x, y)$ over a reference xy-plane placed at z = 0. The topography of the bottom is assumed constant in time. Using the shallow water equations, the water depth h and water flux \mathbf{q} are computed in a reduced dimension

of the problem. Free surface problems that would require a 3D geometry when modeled with the Navier-Stokes equations can be modeled in 2D instead. 2D problems can also be reduced to 1D.

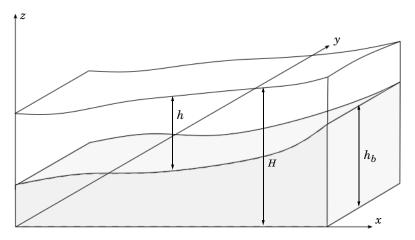


Figure 5-1: An example illustrating a typical configuration for shallow water equations. A water layer of thickness h flows over a nonflat bottom with topography represented by h_b . The total height of the free surface over the reference xy plane at z=0 is represented by H. The gravity points downward (-z direction) and gives rise to a hydrostatic pressure ranging from 0 atm at the free surface to a value of goh at the bottom.

When this physics interface is added, the following default nodes are also added in the Model Builder — Domain Properties, Wall, and Initial Values. Then, from the Physics toolbar, you can add other nodes that implement, for example, boundary conditions. You can also right-click Shallow Water Equations, Time Explicit to select physics features from the context menu.

SETTINGS

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

The Name is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

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

PHYSICAL MODEL

Select a value for **Acceleration of gravity** (SI unit m/s). The default value is g_{const} . It should be a global quantity.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button (5) and select **Advanced** Physics Options in the Show More Options dialog box. Normally these settings do not need to be changed.

Select the CFL number. This CFL number will be used when defining the Cell time scale expression swe.wtc used in the Time-Explicit Solver if the Time stepping is set to From **expressions**. Note that the method will be unstable for CFL numbers larger than 1.



In the COMSOL Multiphysics Reference Manual:

• Time-Explicit Solver

DISCRETIZATION

The Shallow Water Equations, Time Explicit interface uses Nodal discontinuous Lagrange functions with Constant Element order.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Water depth h (SI unit: m) and the Water flux q (SI unit: m^2/s). The names can be changed but the names of fields and dependent variables must be unique within a component.



- Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water **Equations Interface**
- Theory for the Shallow Water Equations Interface



- Dam Breaking on a Column, Shallow Water Equations: Application Library path Subsurface_Flow_Module/Fluid_Flow/dam_break_column_sw
- Tsunami Runup onto a Complex 3D Beach, Monai Valley: Application Library path Subsurface_Flow_Module/Fluid_Flow/monai_runup

Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface

For the Shallow Water Equations interface, the following domain, boundary, edge, point, and pair nodes (listed in alphabetical order) are described in this section:

- Domain Properties
- Domain Source
- Initial Values
- Inlet
- Interior Wall

- Outlet
- Symmetry
- Wall
- Water Source



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

Domain Properties

Use the **Domain Properties** node to set the bottom topography and material properties.

BOTTOM TOPOGRAPHY

The Bottom height (SI unit: m) is defined as a user defined expression. It can depend on the geometry coordinates, but it is expected to be constant in time. The default is set to 0 m.

MATERIAL

The default **Density** ρ (SI unit: kg/m³) is taken **User defined**. Enter a different value or expression. The default is 1000 kg/m³. The density can also be set **From material**. In that case, select the Material to use. By default, the material used is the Domain material. This corresponds to the material currently applied to the domain in question.

The value of the density is not used when solving but to compute the hydrostatic pressure and pressure force.

The **Domain Source** node specifies a momentum source on the right hand-side of the momentum equation

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \left(\mathbf{u} \otimes \mathbf{q} + g \frac{h}{2} \mathbf{I} \right) = -g h_B \nabla h_B + \mathbf{F}$$

This source term can model different effects, such as bottom friction, the Coriolis force, or wind stresses.

Initial Values

The Initial Values node adds an initial value for the water depth and water flux that serve as an initial condition for a transient simulation. If more than one set of initial values is required, add additional Initial Values nodes from the Physics toolbar.

INITIAL VALUES

Select the set of variables to be defined in **Initial values** — **Primitive variables** (the default), or Conservative variables.

For the Water depth, select Specify water depth (the default) or Specify total height.

- For **Specify water depth** provide a value or an expression for the water depth. The default is 0 m.
- For Specify total height provide a value or an expression for the Total height of the water column H. The default is 0 m. When using this option, the initial water depth is calculated as

$$h = \max(0, H - h_b)$$

The variable used to define the water flux \mathbf{q} will depend on the selection of the **Initial** values selection list:

• For **Primitive variables** provide a value or an expression for the components of the velocity **u**. The default is 0 m/s. The initial water depth is then calculated as

$$q = hu$$

• For **Conservative variables** provide a value or an expression for the components of the water flux \mathbf{q} . The default is $0 \text{ m}^2 / \text{s}$.

Use the **Inlet** node to define boundaries where the fluid enters the domain. This condition uses the HLLC Riemann Solver (Ref. 1) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW PROPERTIES

Select the set of variables to be defined in **Input State**—**Primitive variables** (the default), or Conservative variables.

For the Water depth, select User defined (the default), From domain values, or Specify total height.

- For **User defined** provide a value or an expression for the water depth h_0 . The default is 0 m.
- When From domain values is selected, the value of the water depth used to defined the external state is taken from the solution at the boundary. Note that at supercritical inlets both water depth and water flux should be specified.
- For **Specify total height** provide a value or an expression for the **Total height** of the water column H_0 . The default is 0 m. When using this option, the external water depth is calculated as

$$h_0 = \max(0, H_0 - h_b)$$

The variable used to define the water flux \mathbf{q}_0 will depend on the **Input state**:

• For Primitive variables the velocity is provided. If User defined is select, provide a value or an expression for the components of the velocity \mathbf{u}_0 . The default is 0 m/s. The incoming water flux is then calculated as

$$\mathbf{q}_0 = h_0 \mathbf{u}_0$$

If From domain values is selected, the value of the velocity used to defined the external state is taken from the solution at the boundary. Note that at supercritical inlets both water depth and water flux should be specified.

• For Conservative variables the water flux is required. If User defined is select, provide a value or an expression for the components of the water flux \mathbf{q}_0 . The default value is 0 m²/s. If From domain values is selected, the value of the water flux used to defined the external state is taken from the solution at the boundary. Note that at supercritical inlets both water depth and water flux should be specified.

The **Outlet** node defines boundaries where the fluid leaves the domain. This condition uses the HLLC Riemann Solver (Ref. 1) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW PROPERTIES

Select the set of variables to be defined in **Input State** — **Primitive variables** (the default), or Conservative variables.

For the Water depth, select User defined (the default), From domain values, or Specify total height.

- For **User defined** provide a value or an expression for the water depth h_0 . The default is 0 m.
- When From domain values is selected, the value of the water depth used to defined the external state is taken from the solution at the boundary. Note that in supercritical outlets both water depth and water flux should be taken from domain values.
- For Specify total height provide a value or an expression for the Total height of the water column H_0 . The default is 0 m. When using this option, the external water depth is calculated as

$$h_0 = \max(0, H_0 - h_b)$$

The variable used to define the external water flux \mathbf{q}_0 will depend on the **Input state**:

• For Primitive variables the velocity is provided. If User defined is select, provide a value or an expression for the components of the velocity \mathbf{u}_0 . The default is 0 m/s. The outgoing water flux is then calculated as

$$\mathbf{q}_0 = h_0 \mathbf{u}_0$$

If From domain values is selected, the value of the velocity used to defined the external state is taken from the solution at the boundary. Note that in supercritical outlets both water depth and water flux should be taken from domain values.

• For Conservative variables the water flux is required. If User defined is select, provide a value or an expression for the components of the water flux \mathbf{q}_0 . The default value is 0 m²/s. If From domain values is selected, the value of the water flux used to defined the external state is taken from the solution at the boundary. In supercritical outlets both water depth and water flux should be taken from domain values.

Wall

The **Wall** node includes a set of boundary conditions preventing fluid flow in the direction perpendicular to the boundary. A no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, is enforced. Since viscous effects are neglected, no boundary layer develops.

The no-penetration condition is imposed weakly setting the following flux:

$$\Gamma_h \cdot \mathbf{n} = 0$$

$$-\Gamma_q \cdot \mathbf{n} = g \frac{h^2}{2} \mathbf{n}$$



• Theory for the Shallow Water Equations Interface

Symmetry

The **Symmetry** boundary condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. This node sets the same flux condition as the Wall feature.

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at r = 0. The software automatically provides an **Axial Symmetry** node prescribing $\mathbf{u} \cdot \mathbf{n} = 0$ on the axial symmetry boundaries.

Interior Wall

The **Interior Wall** node prevents fluid flow in the direction perpendicular to the boundary. It can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall condition can be used to avoid meshing thin structures by applying a no-penetration condition on interior curves and surfaces instead.

Water Source

The Water Source node specifies a height source in the continuity equation

$$\frac{\partial h}{\partial t} + \nabla \cdot \mathbf{q} \; = \; Q$$

Theory for the Shallow Water Equations Interface

This section describes the theory for the Shallow Water Equations, Time Explicit interface:

- The Shallow Water Equations
- The Numerical Method
- Wave Speed and Flow Regimes
- Forces on Boundaries
- References for the Shallow Water Equations Interfaces

The Shallow Water Equations

Figure 5-2 shows a typical configuration for the flow of fluid in a shallow layer. The upper boundary is referred to as the free surface and the lower boundary of the water layer is referred to as the bottom. The bottom height, h_b , is measured with respect to a reference xy-plane placed at z = 0 and it is assumed to be constant in time. The total height of the free surface is denoted H. The height of the water layer is typically measured in relation to the bottom height and denoted h. In dry regions, h = 0 and $H = h_b$.

The equations of continuity and momentum of incompressible inviscid flow subjected to gravity in the vertical direction ($\mathbf{g} = [0, 0, -g]^T$) are

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{5-1}$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x}$$
 (5-2)

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y}$$
 (5-3)

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g$$
 (5-4)

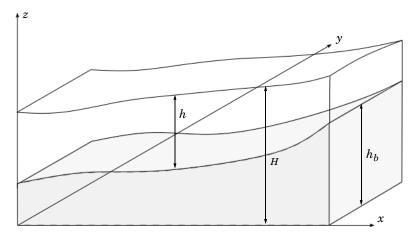


Figure 5-2: An example illustrating a typical configuration for shallow water equations. A water layer of thickness h flows over a nonflat bottom with topography represented by h_b . The total height of the free surface over the reference xy plane at z=0 is represented by H. The gravity points downward (-z direction) and gives rise to a hydrostatic pressure ranging from 0 atm at the free surface to a value of $p = \rho gh$ at the bottom.

Assuming that the water depth h is much smaller than the lateral dimensions of the geometry, the vertical accelerations can be neglected, $\frac{\overline{Dw}}{Dt} = 0$, and Equation 5-4 reduces to the hydrostatic pressure relation

$$\frac{\partial p}{\partial z} = -\rho g \Rightarrow p = \rho g (h + h_b - z)$$
 (5-5)

Both h(x, y) and $h_b(x, y)$ are independent of z, implying that $\frac{\partial p}{\partial x} = \frac{\partial p}{\partial y} = 0$. Equation 5-2 and Equation 5-3 then reduces to

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -g \frac{\partial}{\partial x} (h + h_b)$$
 (5-6)

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -g \frac{\partial}{\partial y} (h + h_b) \tag{5-7}$$

which is the momentum equation of the 2D shallow water equations in nonconservative form. Note that u and v represent the horizontal velocity components averaged over h.

The continuity equation is recovered from Equation 5-1 when assuming no penetration on both the free surface and bottom boundaries:

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} u h + \frac{\partial}{\partial y} v h = 0$$
 (5-8)

See Chapter 2 in Ref. 1 for more details. Equation 5-6, Equation 5-7, and Equation 5-8 can be combined to express the shallow water equations in conservative form

$$\frac{\partial h}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0$$

$$\frac{\partial q_x}{\partial t} + \frac{\partial}{\partial x} \left(uq_x + g \frac{h^2}{2} \right) + \frac{\partial}{\partial y} (uq_y) = -gh \frac{\partial h_b}{\partial x}$$
 (5-9)

$$\frac{\partial q_{y}}{\partial t} + \frac{\partial}{\partial x}(vq_{x}) + \frac{\partial}{\partial y}\left(vq_{x} + g\frac{h^{2}}{2}\right) = -gh\frac{\partial h_{b}}{\partial y}$$
 (5-10)

 q_x and q_y are the components of the water flux in the x and y directions, respectively. The vector $\mathbf{q} = [q_x, q_y, 0]^T$ can be obtained from the horizontally averaged velocity $\mathbf{u} = [u, v, 0]^T$ as

$$\mathbf{q} = \mathbf{u}h \tag{5-11}$$

Two different sets of variables are used in the context of the shallow water equations: the conservative variables h and \mathbf{q} , and the primitive variables h and \mathbf{u} .

The Numerical Method

The physics interface solves the shallow water equations using the Discontinuous Galerkin (DG) method in space together with explicit time stepping. The computations are restricted to transient problems. The basis functions are the nodal discontinuous Lagrange shape functions with constant order.

The numerical method used solves wave problems of the form

$$\mathbf{d}_{\mathbf{a}} \frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \Gamma(\mathbf{w}) = \mathbf{f}$$

When solving the shallow water equations, \mathbf{d}_a is an identity matrix, \mathbf{w} is the vector of conservative variables, Γ represents the conservative fluxes, and **f** includes the source terms:

$$\mathbf{w} = \begin{bmatrix} h \\ \mathbf{q} \end{bmatrix}$$

$$\Gamma(\mathbf{w}) = \begin{bmatrix} \Gamma_h \\ \Gamma_q \end{bmatrix} = \begin{bmatrix} \mathbf{q}^T \\ \mathbf{q} \otimes \mathbf{u} + g\frac{h^2}{2}\mathbf{I} \end{bmatrix}$$

$$\mathbf{f} = \begin{bmatrix} 0 \\ -gh\nabla h_b \end{bmatrix}$$

Here, Γ_h and Γ_q represent the fluxes of the continuity and momentum equations, respectively.

Discontinuous Galerkin methods use shape functions that are continuous in the interior of each mesh element, but discontinuous across element boundaries. A numerical flux must be defined between element boundaries and the dependent variables are not required to be continuous on faces between adjacent mesh elements. The default numerical flux is the Lax-Friedrichs flux, which uses an average of the physical fluxes together with a penalty term.

After discretization in space, the system of equations is integrated in time. The standard procedure is to use an explicit Runge-Kutta method. The physics interface uses the third-order SSP (strong stability preserving) Runge-Kutta method per default.

The time step in explicit computations is limited by the CFL condition; see Time Explicit Integrator in the COMSOL Multiphysics Reference Manual. The maximum stable time step is proportional to the smallest mesh element size h and inversely proportional to the maximum wave speed in the domain. On unstructured meshes with local refinement regions only a few elements are small, yet these dictate the overall time step for the whole problem. In such cases, the use of Local Time Stepping is

advisable. COMSOL Multiphysics provides the **Adams-Bashforth 3 (local)** time stepping method.



Theory for the Wave Form PDE in the COMSOL Multiphysics Reference Manual.

The bottom topography h_b is entered as a user-defined expression. In order to ensure that its gradient can be evaluated and is constant on every element, it is first projected onto the variable swe.hb_linear using linear Lagrangian shape functions. For plotting purposes, the provided expression for h_b is also projected onto the variable swe.hb_constant using the same piecewise discontinuous shape functions as for h. These projections are done in a Stationary study step that must be computed before the Time Dependent study step is used to compute the shallow water equations. When starting a new model from the **Model Wizard**, the stationary study step is added per default when selecting a Time Dependent study.

Wave Speed and Flow Regimes

The fluxes of the momentum and continuity equations, $\Gamma(\mathbf{w})$, provide information about the speed of the waves. The eigenvalues of the Jacobian matrix of the fluxes evaluated at a direction provided by an arbitrary unit vector $\mathbf{n} = [n_x, n_y, 0]^T$ are

$$\lambda_1 = \mathbf{u} \cdot \mathbf{n} - c, \lambda_2 = \mathbf{u} \cdot \mathbf{n}, \lambda_3 = \mathbf{u} \cdot \mathbf{n} + c$$

where c is the wave celerity,

$$c = \sqrt{gh}$$

The eigenvalues of the Jacobian of the fluxes provide information about the velocity at which information is propagated. When $|\mathbf{u} \cdot \mathbf{n}| > c$, the eigenvalues have different sign and information is propagated both upward and downward. If $|\mathbf{u} \cdot \mathbf{n}| < c$, all eigenvalues have the same sign and all waves travel in the same direction.

The Froude number Fr is a dimensionless number typically used to define the flow regime by specifying the ratio of the inertial forces to gravity forces. In case of the Shallow Water Equations, it is defined as

$$Fr = \frac{|\mathbf{u}|}{c}$$

The flow regime can be divided into subcritical flow, Fr < 1, and supercritial flow, Fr > 1. This classification is specially important when defining boundary conditions. In supercritical flows, all characteristics must be specified at inlets and extrapolated from the domain at outlets. In subcritical flows, the characteristics are partially specified from exterior values and partially extrapolated from interior values for both inlets and outlets.

Forces on Boundaries

The physics interface provides variables to compute the pressure force acting on boundaries. In the shallow water equations the pressure is assumed to be hydrostatic

$$p = \rho g(h + h_h - z)$$

The pressure force per unit length on a boundary can be obtained integrating along h

$$\mathbf{F}_{p} = \int_{h}^{0} \rho g z \mathbf{n} dz = \rho g \frac{h^{2}}{2} \mathbf{n}$$

The components of the vector $\mathbf{F}_{\mathbf{p}}$ are available as variables in the Shallow Water Equations, Time Explicit physics interface and can be accessed in 2D using swe.Fpx and swe.Fpy. In 1D only the swe.Fpx component is defined. Note that these variables represent a force per unit length; the total force on a boundary is obtained integrating over the whole boundary.

References for the Shallow Water Equations Interfaces

1. E.F. Toro, Shock capturing methods for free-surface shallow flows, John Wiley & Sons, 2001.

Chemical Species Transport Interfaces

In this chapter:

- The Transport of Diluted Species Interface
- The Transport of Diluted Species in Porous Media Interface
- The Transport of Diluted Species in Fractures Interface
- Theory for the Transport of Diluted Species Interface

In addition, The Reacting Flow in Porous Media Interface is available under the **Chemical Species Transport** branch. It is described in the chapter Multiphysics Interfaces and Couplings.

The Transport of Diluted Species Interface

The Transport of Diluted Species (tds) interface (,), found under the Chemical Species **Transport** branch (is used to calculate the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid, or solid can be handled with this interface. The driving forces for transport can be diffusion by Fick's law, convection when coupled to a flow field, and migration, when coupled to an electric field.

The interface supports simulation of transport by convection and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, c_i , of each species i.

SETTINGS

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

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

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

DOMAIN SELECTION

If any part of the model geometry should not partake in the mass transfer model, remove that part from the selection list.

OUT-OF-PLANE THICKNESS

For 2D components, the **Thickness** field (default value: 1 m) defines a parameter for the thickness of the geometry perpendicular to the two-dimensional cross-section. Both constant and varying thicknesses are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux.

CROSS-SECTIONAL AREA

For 1D components, enter a **Cross-sectional area** A_c (SI unit: m²) to define a parameter for the area of the geometry perpendicular to the 1D component. Both constant and varying areas are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux. The default is 1 m^2

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the check boxes available under Additional transport mechanisms to control other transport mechanisms.

Note: Some of the additional transport mechanisms listed below are only available in certain products. For details see https://www.comsol.com/products/specifications/.

- By default, the **Convection** check box is selected. Clear the check box to disable convective transport.
- Select the Migration in electric field check box to activate transport of ionic species in an electric field. See further the theory section Adding Transport Through Migration.



Transport of ionic species in an electric field is available in a limited set of add-on products. See

https://www.comsol.com/products/specifications/ for more details on availability.

Mass Transport in Porous Media

The Mass transport in porous media check box activates functionality specific to species transport in porous media:

- · Porous Medium
- Unsaturated Porous Medium
- Porous Electrode Coupling

- Volatilization
- Species Source



Note: Mass transport in porous media is only available in a limited set of add-on products. See

https://www.comsol.com/products/specifications/ for more details on availability.

CONSISTENT STABILIZATION

To display this sections, click the **Show** button (**5**) 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_{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 (**5**) 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 (**5**) and select **Advanced Physics Options**. Normally these settings do not need to be changed. Select a **Convective term** — **Nonconservative 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 all settings available in this section, click the **Show** button () and select **Advanced Physics Options.**

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 nonconservative 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 the **Concentration** c by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the Number of species. Use the Add concentration (+) and Remove **concentration** (\equiv) buttons as needed.

FURTHER READING

- Theory for the Transport of Diluted Species Interface
- Numerical Stabilization in the COMSOL Multiphysics Reference Manual.



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



- Effective Diffusivity in Porous Materials: Application Library path COMSOL_Multiphysics/Diffusion/effective_diffusivity
- *Micromixer*: Application Library path COMSOL_Multiphysics/Fluid_Dynamics/micromixer

The Transport of Diluted Species in Porous Media Interface

This interface (), found under the Chemical Species Transport branch (::), is used to calculate the species concentration and transport in free and porous media. The interface is the same as the Transport of Diluted Species interface but it uses other defaults: The Mass Transport in Porous Media property is selected, and a Porous Medium node is added by default. The interface includes reaction rate expressions and solute sources for modeling of species transport and reaction in porous media.

This interface is dedicated to modeling transport in porous media, including immobile and mobile phases, where the chemical species may be subjected to diffusion, convection, migration, dispersion, adsorption, and volatilization in porous media. It

supports cases where either the solid phase substrate is exclusively immobile, or when a gas-filling medium is also assumed to be immobile.

It applies to one or more diluted species or solutes that move primarily within a fluid that fills (saturated) or partially fills (unsaturated) the voids in a solid porous medium. The pore space not filled with fluid contains an immobile gas phase. Models including a combination of porous media types can be studied.

The main feature nodes are the **Porous Medium** and **Unsaturated Porous Medium** nodes, which add the equations for the species concentrations and provide an interface for defining the properties of the porous media, as well as additional properties governing adsorption, volatilization, dispersion and diffusion, migration, and the velocity field to model convection.

The physics interface can be used for stationary and time-dependent analysis.

When this physics interface is added, these default nodes are also added to the **Model** Builder — Porous Medium, No Flux (the default boundary condition), and Initial Values. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, reaction rate expressions, and species sources. You can also right-click Transport of Diluted Species in Porous Media to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as The Transport of Diluted Species Interface.

FURTHER READING

Web link:



- Mass Balance Equation for Transport of Diluted Species in Porous Media
- Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface
- Variably Saturated Flow and Transport Sorbing Solute: Application Library path



Subsurface_Flow_Module/Solute_Transport/sorbing_solute

https://www.comsol.com/model/variably-saturated-flow-and-transp ort-sorbing-solute-490

Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the Physics ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).



- To add a node, go to the **Physics** toolbar, no matter what operating system you are using.
- Contextual subnodes (attributes) are available by clicking the parent node in the Model Builder, and then selecting the subnode from the Attributes menu.

- Adsorption
- Concentration
- Continuity on Interior Boundaries
- Dispersion
- Electrode Surface Coupling
- Equilibrium Reaction
- Fast Irreversible Surface Reaction
- Fluid
- Flux
- Flux Discontinuity
- Fracture
- Gas
- Inflow
- Initial Values
- Line Mass Source
- Liquid
- Mass-Based Concentrations
- No Flux
- Open Boundary
- Out-of-Plane Flux
- Outflow
- Partition Condition

- Periodic Condition
- Point Mass Source
- Porous Matrix
- Porous Medium
- Porous Electrode Coupling
- Reaction Coefficients
- Reactions
- Species Source
- Surface Reactions
- Surface Equilibrium Reaction
- Symmetry
- Thin Diffusion Barrier
- Thin Impermeable Barrier
- Transport Properties
- Unsaturated Porous Medium
- Volatilization

Some features require certain add-on modules. For details see https://www.comsol.com/products/specifications/



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



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

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.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the Temperature list.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the Velocity field list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select Material, and a Fluid material to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the Fluid diffusion coefficient list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when Calculate transport properties is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the Fluid diffusion coefficient list.

For **User defined**, enter a value or expression for the **Fluid diffusion coefficient** $D_{
m c}$ of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the Migration in electric field 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 **Full** and type in the value of expression of the mobility $u_{\rm m.c.}$

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based on the Nernst-Einstein relation) is taken from Model Inputs section.

Note that the migration in electric fields feature is only available in some COMSOL products. See details: https://www.comsol.com/products/specifications/.

EXAMPLE MODELS



• Separation Through Dialysis: Application Library path Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis Web link:

https://www.comsol.com/model/separation-through-dialysis-258



• Transport in an Electrokinetic Valve: Application Library path Microfluidics Module/Fluid Flow/electrokinetic valve

Web link: https://www.comsol.com/model/electrokinetic-valve-603

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/m³) and mass fractions (dimensionless) for all species.

MIXTURE PROPERTIES

The default Solvent density $ho_{
m solvent}$ is taken From material. For User defined, enter a value or expression manually. Define the Molar mass of each species, which is needed to calculate the mass-based concentration.

Reactions

Use the Reactions node to account for the consumption or production of species through chemical reactions. Define the rate expressions as required.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

REACTION RATES

Add a rate expression R_i (SI unit: mol/(m³·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 https://www.comsol.com/products/specifications/ for more details on availability.

When specifying reaction rates for a species in porous media, the specified reaction rate may have the basis of the total volume, the pore volume, or the volume of a particular phase.

- For **Total volume**, the reaction expressions in mol/(m³·s) are specified per unit volume of the model domain (multiplied by unity).
- For **Pore volume**, the reaction expressions in $mol/(m^3 \cdot s)$ are specified per unit volume of total pore space. The reaction expressions will be multiplied by the domain porosity, ε_n . (ε_n equals unity for nonporous domains.)

- For **Liquid phase**, the reaction expressions in mol/(m³·s) are specified per unit volume of liquid in the pore space. The expressions will be multiplied by the liquid volume fraction θ . (θ equals $\varepsilon_{\rm p}$ for Saturated Porous Media domains).
- For **Gas phase**, the expressions are multiplied by the gas volume fraction $a_v = \varepsilon_p \theta$. $a_{\rm v}$ equals 0 for Saturated Porous Media domains.

FURTHER READING

See the theory chapter on chemical species transport, starting with the section Mass Balance Equation.

• Fine Chemical Production in a Plate Reactor: Application Library

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Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_T ransfer/plate_reactor

Web link:

https://www.comsol.com/model/fine-chemical-production-in-a-pla te-reactor-8589

No Flux

This node is the default boundary condition on exterior boundaries. It should be used on boundaries across which there is no mass flux, typically solid walls where no surface reactions occur. The condition applied for each species corresponds to

$$-\mathbf{n} \cdot (-D\nabla c) = 0$$

where **n** denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the no flux condition is:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathbf{m}} F c \nabla \phi) = 0$$

CONVECTION

By default, the feature prescribes a vanishing flux due to diffusion and migration in an electric field. This is the appropriate no flux condition when the relative convective velocity at the boundary is zero. When the fluid velocity at the boundary is not equal to that of the boundary, it is often convenient to prescribe the total flux including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the no flux condition prescribed is

$$-\mathbf{n}\cdot(-D\nabla c+\mathbf{u}c)=0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{m}Fc\nabla\phi + \mathbf{u}c) = 0$$

when migration of ionic species is included.

Inflow

Use this node to specify all species concentrations at an inlet boundary.

If you want to specify the concentration of a subset of the partaking species, this can be done by using the Concentration node instead.

For the **Electroanalysis** interface, this node is available when you select the **Convection** check box on the physics interface **Settings** window.

CONCENTRATION

For the concentration of each species $c_{0,c}$ (SI unit: mol/m³), enter a value or expression.

BOUNDARY CONDITION TYPE

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints.

The other option, Flux (Danckwerts) can be used when the concentration at the boundary is not known, or when it varies in a non-trivial manner. This may, for example, be useful when reactions with high reaction rates occur in the vicinity of the inlet. In this case the concentration far upstream of the boundary is instead prescribed. The Flux (Danckwerts) condition prescribes the total flux defined by the upstream concentration and the fluid velocity at the boundary.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (**a**) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the COMSOL Multiphysics Reference Manual.

FURTHER READING

See the theory chapter in the section Danckwerts Inflow Boundary Condition.

Outflow

Apply this condition at outlets boundaries where species should be transported out of the model domain by fluid motion or by an electric field (in the case of ions). It is assumed that convection and migration (in an electric field) are the dominating transport mechanisms across the boundary, and therefore that the diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D\nabla c) = 0$$

Note that the **Convection** or the **Migration in electric field** transport mechanisms needs to be included for this node to be available.

Concentration

This condition node adds a boundary condition for the species concentration. For example, a $c = c_0$ condition specifies the concentration of species c.

CONCENTRATION

Individually specify the concentration for each species. Select the 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 in the COMSOL Multiphysics Reference Manual.

Flux

This node can be used to specify the species molar flux across a boundary. The flux can for example occur due to chemical reactions or a phase change at the boundary. The flux can also represent the transport to or from a surrounding environment currently not included model.

The prescribed flux of a species c is by default defined as

$$-\mathbf{n}\cdot(-D\nabla c) = J_0$$

where **n** denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathbf{m}}Fc\nabla\phi) = J_0$$

The flux prescribed, J_0 , can include any arbitrary user-specified expression. It can be constant or a function of a dependent variable or independent variable. Common examples are a flux dependent of the concentration, temperature, pressure or the electric potential ϕ .

CONVECTION

By default, the flux due to diffusion and migration in an electric field is prescribed. This is the appropriate flux condition when the relative velocity at the boundary is zero. When the fluid velocity is not equal to that of the boundary, it is often convenient to prescribe the total flux, including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the prescribed flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = J_0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathbf{m}} F c \nabla \phi + \mathbf{u}c) = J_0$$

when migration of ionic species is included.

INWARD FLUX

Select the Species check box for the species for which to specify the flux, and enter a value or expression for the inward flux in the corresponding field. Use a minus sign when specifying a flux directed out of the system. To use another boundary condition for a specific species, click to clear the check box for that species.

External convection

Set Flux type to External convection to prescribe a flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$J_0 = k_c(c_b - c)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain.

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric, that is, where there is no mass flux across the boundary.

This boundary condition is identical to that of the No Flux node.

Flux Discontinuity

This node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n} \cdot [(\mathbf{J} + \mathbf{u}c)_{\mathbf{u}} - (\mathbf{J} + \mathbf{u}c)_{\mathbf{d}}] = N_0 \qquad \mathbf{J} = -D\nabla c$$

where the value N_0 (SI unit: mol/(m²·s)) specifies the jump in total flux at the boundary. This can be used to model a boundary source, for example a surface reaction, adsorption or desorption.

FLUX DISCONTINUITY

In this section the jump in species flux (or surface source) is specified.

Select the Species 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.

Partition Condition

The **Partition Condition** node can be used to prescribe the relation between the concentration of a solute species in two adjoining immiscible phases. It can for example be used on interior boundaries separating two liquid phases, a gas-liquid interface, or on a boundary separating a liquid phase and a solid or porous media.

Select **Partition coefficient** from the **Relation** list to prescribe a linear relationship between the concentration on either side of a boundary. For a species concentration c_i , the ratio between the concentration on the upside and on the downside of the boundary ($c_{i,u}$ and $c_{i,d}$ respectively) is then defined in terms of a partition coefficient K_i in the manner of

$$K_i = \frac{c_{i, u}}{c_{i, d}}$$

Use the associated input field to prescribe the partition coefficient for each species.

Select User defined from the Relation list to set up a nonlinear relation between the up and downside concentrations. For such relations $f(c_i)_n = f(c_i)_d$, where $f(c_i)_n$ is the expression enforced on the upside. Use the associated input fields to enter the upside and downside expressions for each species.

The up and downside of the selected boundary is indicated with a red arrow in the Graphics window. The arrow points from the downside into the upside. Select the **Reverse direction** check box to reverse the direction of the arrow on the selected boundary, and update the definition of the up and downside concentrations accordingly.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

FURTHER READING

For an example of using a partition condition, see this application example:



Separation Through Dialysis: Application Library path Chemical Reaction Engineering Module/Mixing and Separation/dialysis

Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the mass transport between two sets of boundaries. The node prescribes continuity in the concentration and the mass flux between the "source" and the "destination" side respectively. Note that these names are arbitrary and does not influence the direction in which mass is transported. It is dictated by mass transfer equations in the adjacent domains.

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

For more complex geometries, it might be necessary to add the Destination Selection 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

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



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SELECTION

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

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

SPECIES SOURCE

Enter the source strength, $q_{l,c}$, for each species (SI unit: mol/(m·s)). A positive value results in species injection from the line into the computational domain, and a negative value means that the species is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Point Mass Source

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



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SPECIES SOURCE

Enter the source strength, $q_{p,c}$, for each species (SI unit: mol/s). A positive value results in species injection from the point into the computational domain, and a negative value means that the species is removed from the computational domain.

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

FURTHER READING

See the section Mass Sources for Species Transport.

Open Boundary

Use this node to set up mass transport across boundaries where both convective inflow and outflow can occur. On the parts of the boundary where fluid flows into the domain, an exterior species concentration is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the Outflow node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Transport of Diluted Species interface.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EXTERIOR CONCENTRATION

Enter a value or expression for the **Exterior concentration**.

Thin Diffusion Barrier

Use this boundary condition to model a thin layer through which mass is transported by diffusion only. The node is applicable on interior boundaries and can be used to avoid meshing thin structures.

THIN DIFFUSION BARRIER

Specify the Layer thickness, d_s , and input a Diffusion coefficient, $D_{s,c}$, for each of the species included.

Thin Impermeable Barrier

This feature models a thin mass transfer barrier. It is available on interior boundaries and introduces a discontinuity in the concentration across the boundary. On each side, a no-flux condition is prescribed for the mass transport implying that it acts as a barrier. The feature can be used to avoid meshing thin structures.

Solving a model involving coupled fluid flow and mass transfer, the Thin Impermeable Barrier feature can be combined with an Interior Wall feature in order to model a thin solid wall.

Equilibrium Reaction

Use this node to model a reaction where the kinetics is so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the reaction rate $R_{\rm eq}$) 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.

> • A necessary requirement for this is feature to be available is that two or more species are solved for by the interface.



• This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EQUILIBRIUM CONDITION

The list defaults to **Equilibrium constant** or select **User defined**. For either option, the Apply equilibrium condition on inflow boundaries check box is selected by default.

For **Equilibrium constant**, enter an **Equilibrium constant** $K_{\rm eq}$ (dimensionless). Also enter a value or expression for the **Unit activity concentration** C_{a0} (SI unit: mol/m³). Selecting **Equilibrium constant** defines an equilibrium condition based on the stoichiometric coefficients, the species activities, and the law of mass action.

For User defined, enter an Equilibrium expression $E_{\rm eq}$ (dimensionless).

STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient v_c (dimensionless). The default is 0. Use negative values for reactants and positive values for products in the modeled reaction.

Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium** Reaction node.

Surface Reactions

The Surface Reactions node can be used to account for the species boundary flux due to chemical reactions occurring on a surface (heterogeneous reactions). For a domain species participating in a surface reaction, the boundary flux corresponds to the reaction rate at the surface.

SURFACE REACTION RATE

Specify the surface reaction rate J_0 of each species resulting from the reactions. Note that if you have the Chemistry interface available, provided with the Chemical

Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down menu.

FURTHER READING

For an example of using the Surface Reactions node, see this application example:



Chemical Vapor Deposition of GaAs: Application Library path Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Tran sfer/gaas_cvd

Surface Equilibrium Reaction

Use this node to model an equilibrium reaction on a boundary (surface). The settings for this node are similar to Equilibrium Reaction. Note that a necessary requirement for this is feature to be available is that two or more species are solved for by the interface.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Fast Irreversible Surface Reaction

This boundary node defines an irreversible reaction where the kinetics is so fast that the only factor limiting the reaction rate is the transport of a species to the reacting surface.

The node will set the Rate limiting species concentration to zero at the boundary, and balance the fluxes of the species participating in the reaction and the current densities according to the Stoichiometric Coefficients settings.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Electrode Coupling

Use this node to add a molar source in a domain that is coupled to one or multiple Porous Electrode Reaction nodes of an Electrochemistry Interface.

The molar source is calculated from the number of electrons, stoichiometric coefficients, and volumetric current densities of the coupled porous electrode reactions specified in the Reaction Coefficients subnodes.

In the Transport of Concentrated Species interface, the molar sources (or sinks) are multiplied by the species molar masses to obtain the corresponding mass sources.

Additional Reaction Coefficients subnodes are available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Note that if you are also modeling the momentum transport and expect a 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.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Reaction Coefficients

Add this node to the Electrode Surface Coupling and Porous Electrode Coupling features to define molar fluxes and sources based on electrode current densities in an **Electrochemistry** interface.

The molar flux or source is proportional to the stoichiometric coefficients and the current density according to Faraday's law.

Current densities from **Electrode Reaction** (i_{loc} , SI unit: A/m²) or **Porous Electrode Reaction** nodes $(i_v, SI \text{ unit: A/m}^3)$ of any **Electrochemistry** interface in the model are available for selection as the **Coupled reaction**, and user-defined expressions are also supported.

Enter the **Number of participating electrons** n_m (dimensionless) and the **Stoichiometric coefficient** v_c (dimensionless) as explained in the theory section linked below.

Use multiple subnodes to couple to multiple reactions.

Electrode Surface Coupling

Use this node to define a flux boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flux is proportional to the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficients subnodes.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass flux over the boundary, which is often the case for gas diffusion electrodes, you need to also add a corresponding Electrode Surface Coupling node in the Fluid Flow interface.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Species transport through a porous medium is affected both by properties of the fluid phase, and as well as properties of the solid matrix. These properties are defined in the Fluid and Porous Matrix subnodes respectively. The Porous Medium node supports material properties using a Porous Material node (described in the COMSOL Multiphysics Reference Manual), where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the **Porous Medium** to account for the corresponding transport mechanism.

Use this node to specify the mass transfer in the mobile fluid solvent filling the pores of a porous medium. It is used as a subnode to Porous Medium.

MODEL INPUTS

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

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

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select Material, and a Fluid material to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the Fluid diffusion coefficient list.

Select Chemistry to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when Calculate transport properties is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the Fluid diffusion coefficient list.

For User defined, enter a value or expression for the Fluid diffusion coefficient $D_{\mathrm{F,i}}$ of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an Effective diffusivity model to account for the reduced diffusivity. The available models are Millington and Quirk model (the default), Bruggeman model, Tortuosity model, or No correction. For Tortuosity model, enter a value for the tortuosity $\tau_{F,i}$ (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: https://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.

- For **User defined**, enter a value or expression for the **Electric potential** V. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the Mobility is set to be calculated based on the species effective diffusivity and the temperature using the Nernst-Einstein relation. For User defined, select the appropriate scalar or tensor type — Isotropic, Diagonal, Symmetric, or Full — and type in the value or expression of the effective mobility $u_{\text{me.i}}$.

Enter the **Charge number** z_c for each species.

Porous Matrix

This node sets the porosity when modeling transport of diluted species in a Porous Medium or a Unsaturated Porous Medium.

The default **Porosity** ε_{p} of the solid matrix is taken **From material**. The Porous Matrix node supports the use of a **Porous Material** node, where the porosity is defined in the manner of

$$\varepsilon_{\rm p} = 1 - \sum_{i} \theta_{\rm s, i} - \sum_{i} \theta_{\rm imf, i}$$

where $\theta_{s,i}$ and $\theta_{imf,i}$ are the porosities of the **Solid** and **Immobile Fluids** subnodes under the Porous Material node.

Select From pellet bed densities to compute the porosity using the (dry bulk) Bed density ρ_b and the (single phase) Pellet density ρ_{pe} . The porosity is then defined from

$$\varepsilon_{\rm p} = 1 - \frac{\rho_{\rm b}}{\rho_{\rm pe}}$$

For **User defined**, enter a value or expression for the porosity.

Dispersion

Local variations in the velocity as the fluid flows around solid particles lead to mechanical mixing, referred to as dispersion. Use this feature to account for dispersion in a Porous Medium or a Unsaturated Porous Medium

This subfeature is available when both the Mass transfer in porous media mass transfer check box and the Convection check box are 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_D (SI unit: m²/s) for each species separately. When not selected the same dispersion tensor $D_{\rm D}$ is used for all species.

Select an option from the **Dispersion tensor** list — **Dispersivity** or **User defined**.

Select **Dispersivity** to specify the dispersion in terms of dispersivities (SI unit: m). Select an option from the Dispersivity model list: Isotropic (the default) or Transverse isotropic based on the properties of the porous media. For isotropic porous media, specify the longitudinal and transverse dispersivities. For transverse isotropic porous media, specify the longitudinal, horizontal transverse, and vertical transverse dispersivities.

For **User defined**, specify the dispersion components in terms of constants or expressions. Select Isotropic, Diagonal, Symmetric, or Full to enable the appropriate tensor components.

Unsaturated Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

Use this node to model the concentration of diluted species transported by a liquid (mobile fluid phase) in a partially filled solid porous medium. The interstices of the porous medium contains the liquid carrier phase and gas pockets. Apart from convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and volatilization.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The properties of each phase present are defined using the Liquid, the Gas, and the Porous Matrix subnodes respectively. The Unsaturated Porous Medium node supports material properties using a Porous Material node (described in the COMSOL Multiphysics Reference Manual), where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the Unsaturated Porous Medium to account for the corresponding transport mechanism.

Liquid

Use this node to specify the mass transfer in the mobile liquid solvent present in the pores of the Unsaturated Porous Medium.

MODEL INPUTS

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

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

SATURATION

Select **Saturation** or **Liquid volume fraction** from the list.

For **Saturation**, enter a value for s (dimensionless) between 0 and 1. The liquid volume fraction is then computed from the saturation and porosity as $\theta_1 = \varepsilon_p s$.

For **Liquid volume fraction**, enter a value for θ_1 (dimensionless) between 0 and the value of the porosity.

Select a Liquid fraction time change: Liquid fraction constant in time (the default), Time change in liquid fraction, or Time change in pressure head.

- For Time change in fluid fraction, enter $d\theta/dt$ (SI unit: 1/s).
- For Time change in pressure head, enter dH_p/dt (SI unit: m/s) and a Specific moisture capacity C_m (SI unit: 1/m). If a Darcy's Law interface is included in the component, the time change in pressure head solved for can be selected.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent liquid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select Material, and a Liquid material to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Liquid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when Calculate transport properties is selected on the interface level of a Chemistry interface. All

defined diffusion coefficients are available for selection in the Liquid diffusion coefficient list.

For User defined, enter a value or expression for the Liquid diffusion coefficient D_{Li} of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an Effective diffusivity model, liquid to account for the reduced diffusivity in the liquid. The available models are Millington and Quirk model (the default), Bruggeman model, Tortuosity model, or No correction. For Tortuosity **model**, enter a value for the tortuosity τ_{Li} (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. For details see: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

- For **User defined**, enter a value or expression for the **Electric potential** V. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the Nernst-Einstein relation. For User defined, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value or expression of the effective mobility $u_{\text{me.i.}}$

Enter the **Charge number** z_c for each species.

Gas

Use this node to specify the mass transfer in the gas phase present in the pores of the Unsaturated Porous Medium.

DIFFUSION

The settings for the diffusion of each species in the gas phase are identical to those in the Liquid subnode.

VOLATILIZATION

Enter a value for the volatilization isotherm $k_{G,c}$ (dimensionless) for each species.

Adsorption

Use this node to model adsorption of the (fluid phase) solute species onto the surface of the porous matrix. It is available as a subnode to the Porous Medium and the Unsaturated Porous Medium nodes.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

MATRIX PROPERTIES

The density of the porous media is needed when modeling adsorption to the surface of the porous matrix. Choose to input either the **Dry bulk density** ρ , or the **Solid phase density** ρ_s . The former is the density of the porous matrix including empty pores, while the latter corresponds to the density of the pure solid phase. The density can be defined from the domain material by selecting **From material**, or from a user defined expression. When a **Porous Material** is used on the selection, the density will be requested from a Solid subfeature. Several Solid features can be used to model a homogeneous mixture of several solid components.

ADSORPTION

Select an Adsorption isotherm — Langmuir, Freundlich, Toth, BET, or User defined to specify how to compute $c_{\rm P}$, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

For Langmuir:

$$c_{\rm P} = c_{\rm Pmax} \frac{K_{\rm L}c}{1 + K_{\rm L}c} \quad , \quad K_P = \frac{\partial c_{\rm P}}{\partial c} = \frac{K_{\rm L}c_{\rm Pmax}}{\left(1 + K_{\rm L}c\right)^2}$$

Enter a Langmuir constant $k_{L,c}$ (SI unit: m³/mol) and an Adsorption maximum $c_{p,\text{max,c}}$ (SI unit: mol/kg).

• For Freundlich:

$$c_{\mathrm{P}} = K_{\mathrm{F}} \left(\frac{c}{c_{\mathrm{ref}}}\right)^{N}$$
 , $K_{P} = \frac{\partial c_{\mathrm{P}}}{\partial c} = N \frac{c_{\mathrm{P}}}{c}$

Enter a Freundlich constant $k_{
m F,c}$ (SI unit: mol/kg), a Freundlich exponent $N_{
m F,c}$ (dimensionless), and a **Reference concentration** $c_{\text{ref,c}}$ (SI unit: mol/m³).

• For Toth:

$$c_{\rm P} = c_{\rm Pmax} \frac{b_{\rm T} c}{\left(1 + (b_{\rm T} c)^{N_{\rm T}}\right)^{1/N_{\rm T}}}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = c_{\text{Pmax}} b_{\text{T}} (1 + (b_{\text{T}} c)^{N_{\text{T}}})^{-\left(1 + \frac{1}{N_{\text{T}}}\right)}$$

Enter a **Toth constant** $b_{\mathrm{T,c}}$ (SI unit: m $^3/\mathrm{mol}$), a **Toth exponent** $N_{\mathrm{T,c}}$ (dimensionless), and an Adsorption maximum $c_{p,\max,c}$ (SI unit: mol/kg).

• For BET (Brunauer-Emmett-Teller):

$$c_{\rm P} = \frac{K_{\rm B} c_0 c}{(c_{\rm S} - c) \left(1 + (K_{\rm B} - 1) \frac{c}{c_{\rm S}}\right)}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = \frac{K_B c_0 c_S ((K_B - 1)c^2 + c_S^2)}{(c - c_S)^2 (c_S + (K_P - 1)c)^2}$$

Enter a BET constant $K_{\mathrm{B,c}}$ (dimensionless), a Monolayer adsorption capacity $c_{0,\mathrm{c}}$ (SI unit: mol/kg), and an **Saturation concentration** $c_{S,c}$ (SI unit: mol/m³).

• For User defined enter an Adsorption isotherm $c_{\mathrm{P,c}}$ (SI unit: mol/kg):

$$c_{\rm P} = f(c)$$

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.

Volatilization

This feature is available when the Mass transfer in porous media check box is selected on the Settings window for the physics interface.

Use this feature to model mass transfer at the boundary due to volatilization. The species dissolved in the liquid are assumed to be vaporized at the boundary, and transported into the surrounding bulk region due to convection and diffusion. The mass transfer at the boundary is defined as

$$-\mathbf{n} \cdot \mathbf{J}_{c} = -h_{c}(k_{G,c}c - c_{Gatm,c})$$

where $h_{\rm c}$ is the mass transfer coefficient, $k_{\rm G,c}$ the volatilization coefficient, and $c_{\rm Gatm,c}$ the concentration in the surrounding atmosphere.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

VOLATILIZATION

Enter a Mass transfer coefficient h_c defining the transfer into the surrounding media. This can be given by boundary layer theory. When assuming that no convective flow is present in the surrounding, the mass transfer coefficient can be defined from the gas diffusion coefficient D_{Gc} and the thickness of the diffusion layer d_{s} in the manner of

$$h_{\rm c} = \frac{D_{G\rm c}}{d_{\rm s}}$$

Also give the atmospheric concentration for each species, $c_{\text{Gatm.c}}$. The **Volatilization** coefficient $k_{G,c}$ for each species are taken from the adjacent Unsaturated Porous Medium domain.

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/(m³·s)) for each of the species solved for. Enter a value or expression in the field of the corresponding species.

Hygroscopic Swelling

The Hygroscopic Swelling multiphysics coupling node () is used for moisture concentration coupling between the Solid Mechanics interface and either the Transport of Diluted Species or Transport of Diluted Species in Porous Media interfaces.

Hygroscopic swelling is an effect of internal strain caused by changes in moisture content. This volumetric strain can be written as

$$\varepsilon_{\rm hs} = \beta_{\rm h} M_{\rm m} (c_{\rm mo} - c_{\rm mo,ref})$$

where $\beta_{\rm h}$ is the coefficient of hygroscopic swelling, $M_{
m m}$ is the molar mass, $c_{
m mo}$ is the moisture concentration, and $c_{
m mo,ref}$ is the strain-free reference concentration.

This feature requires a license of either the MEMS Module or the Structural Mechanics Module. The multiphysics feature will appear automatically if both the Transport of Diluted Species and the Solid Mechanics interfaces are added to the same component. For the most current information about licensing, please see See https://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 Branch in the COMSOL Multiphysics Reference Manual.

Out-of-Plane Flux

The out-of-plane flux node is used to prescribe a flux in an out-of-plane domain, and it can be used to reduce a model geometry to 2D, or even 1D, when the concentration variation is small in one or more directions. This could be the case for example when the object to model is thin or slender. Figure 6-1shows examples of possible situations in which this type of geometry reduction can be applied.

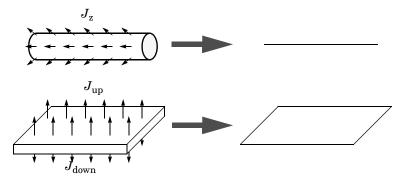


Figure 6-1: Geometry reduction from 3D to 1D (top) and from 3D to 2D (bottom).

For a 1D component this node adds a single out-of-plane molar flux $J_{0,z,i}$ for species i. For a 2D component two fluxes can be prescribed for each species; $J_{0,u,i}$ for the upside of the domain, and $J_{0,\mathbf{d},i}$ for the downside of the domain.

The fluxes are added as a source contribution to the right-hand side of the transport equation. For example, in 2D components with diffusion, convection and out-of-plane flux present, mass transfer of species i is defined by the mass conservation equation

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i + S_{\mathbf{opf}, i} \qquad , \tag{6-1}$$

where $S_{\mathrm{opf},i}$ is the out-of-plane source for species i

$$S_{\text{opf},i} = \frac{J_{0,i}}{d_z} = \frac{J_{0,u,i} + J_{0,d,i}}{d_z}.$$

For external convection on the upside and the downside of the domain, the out-of-plane flux is

$$J_{0, i} = k_{c, \mathbf{u}, i} (c_{b, \mathbf{u}, i} - c_i) + k_{c, \mathbf{d}, i} (c_{b, \mathbf{d}, i} - c_i)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain. The prescribed flux, J_0 , can include any arbitrary user-specified expressions. It can be a constant or a function of a dependent variable or independent variables.

UPSIDE INWARD FLUX

For 1D components, enter the **cross-sectional perimeter** P_c to get the out-of-plane flux

$$J_{0,i} = P_c J_{0,Z,i}$$
.

The default value of P_c is the circumference. Either keep the default value, for a circular cross-section shape, or edit the value to get a user-defined shape of the out-of-plane cross-section.

The available flux type options are General inward flux and External convection. Select the **Species** check box for the species for which to specify the flux, and enter a value or expression for the inward flux in the corresponding field. Use a minus sign when specifying a flux directed out of the system. To use another boundary condition for a specific species, click to clear the check box for that species.

Set Flux type to External convection to prescribe a flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$J_0 = k_{\rm c}(c_{\rm b} - c)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain.

DOWNSIDE INWARD FLUX

The available options are General inward flux and External convection. The settings are the same as for the Upside Inward Flux section.

FURTHER READING

For an example of using the Out-of-Plane Flux node, see this application example:



Mass Transfer from a Thin Domain: Application Library path Chemical_Reaction_Engineering_Module/Tutorials/thin_domain

Fracture

Use this node to model mass transport along thin fractures in porous media. The node assumes that the transport in the tangential direction along the fracture is dominant, as a result of lower flow resistance.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

FRACTURE PROPERTIES

Specify a value for the **Fracture thickness** $d_{\rm fr}$.

MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the Boundary material is used.

Specify the **Porosity**, \mathcal{E}_{p} (dimensionless) of the porous matrix. This is by default taken From material. Select User defined to instead enter a different value.

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** is the similar to the settings for the diffusion coefficients in the Fluid node. The Dispersion settings are identical to the ones in the Dispersion node.

The Transport of Diluted Species in Fractures Interface

The Transport of Diluted Species in Fractures (dsf) interface (1), found under the Chemical Species Transport branch (🐏), is used to model the transport of a solute species along thin porous fractures, taking into account diffusion, dispersion, convection, and chemical reactions. The fractures are defined by boundaries and the solute species is assumed to be present in a solvent.

The interface supports simulation of species transport along boundaries in 2D and 3D, and axisymmetric components in 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.



This interface is only available in a limited set of add-on products. For a detailed overview of which interfaces are available in each product, visit https://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 dsf.

BOUNDARY SELECTION

If model geometry includes boundaries that should not be included in the mass transfer simulation, remove those from the selection list.

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the **Convection** check box, available under Additional transport mechanisms, to control whether to also include convective transport.

CONSISTENT STABILIZATION

To display this sections, click the **Show** button (**5**) and select **Stabilization**. Use this section to control the application of the available consistent stabilization methods; Streamline diffusion and Crosswind diffusion.

- 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_{\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 (**5**) 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.

DISCRETIZATION

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

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. A dependent variable name 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

- Mass Transport in Fractures in the theory section.
- 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 2-4 for links to common sections and Table 2-5 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Boundary, Edge, Point, and Pair Nodes for the Transport of Diluted Species in Fractures Interface

The Transport of Diluted Species in Fractures Interface has the following boundary, edge, point, and pair nodes, listed in alphabetical order, available from the Physics ribbon toolbar (Windows users), Physics context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- Adsorption
- Concentration
- Flux
- Fracture
- Inflow

- Initial Values
- No Flux
- Outflow
- Reactions
- Species Source

Use this node to model adsorption of the fluid phase species onto the porous media surface of the fracture.

MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Domain material** is used. The density of the porous media is needed when modeling adsorption to the surface of the porous matrix. By default **Density** ρ is set to from domain material.

ADSORPTION

Select an Adsorption isotherm — Langmuir (the default), Freundlich, Toth, BET, or User **defined** to specify how to compute $c_{\rm P}$, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

· For Langmuir:

$$c_{\rm P} = c_{\rm Pmax} \frac{K_{\rm L}c}{1 + K_{\rm L}c} \qquad \frac{\partial c_{\rm P}}{\partial c} = \frac{K_{\rm L}c_{\rm Pmax}}{(1 + K_{\rm L}c)^2}$$

Enter a Langmuir constant $k_{\rm L,c}$ (SI unit: m³/mol) and an Adsorption maximum $c_{\text{p,max,c}}$ (SI unit: mol/kg):

• For Freundlich:

$$c_{\rm P} = K_{\rm F} \left(\frac{c}{c_{\rm rof}}\right)^N \quad \frac{\partial c_{\rm P}}{\partial c} = N \frac{c_{\rm P}}{c}$$
 Freundlich

Enter a Freundlich constant $k_{\mathrm{F,c}}$ (SI unit: mol/kg), a Freundlich exponent $N_{\mathrm{F,c}}$ (dimensionless), and a Reference concentration $c_{
m ref,c}$ (SI unit: mol/m³).

• For Toth:

$$c_{\rm P} = c_{\rm Pmax} \frac{b_{\rm T} c}{(1 + (b_{\rm T} c)^{N_{\rm T}})^{1/N_{\rm T}}}$$

and

$$\frac{\partial c_{P}}{\partial c} = c_{Pmax} b_{T} (1 + (b_{T}c)^{N_{T}})^{-\left(1 + \frac{1}{N_{T}}\right)}$$

Enter a **Toth constant** $b_{\mathrm{T,c}}$ (SI unit: $\mathrm{m^3/mol}$), a **Toth exponent** $N_{\mathrm{T,c}}$ (dimensionless), and an Adsorption maximum $c_{\mathrm{p,max,c}}$ (SI unit: mol/kg).

• For BET (Brunauer-Emmett-Teller):

$$c_{\rm P} = \frac{K_{\rm B}c_0c}{(c_{\rm S} - c)\Big(1 + (K_{\rm B} - 1)\frac{c}{c_{\rm S}}\Big)}$$

and

$$\frac{K_{\rm B}c_0c_{\rm S}((K_{\rm B}-1)c^2+c_{\rm S}^2)}{(c-c_{\rm S})^2(c_{\rm S}+(K_{\rm B}-1)c)^2}$$

Enter a BET constant $K_{\mathrm{B,c}}$ (dimensionless), a Monolayer adsorption capacity $c_{0,\mathrm{c}}$ (SI unit: mol/kg), and an Saturation concentration $c_{S,c}$ (SI unit: mol/m³).

• For User defined:

$$c_{\mathbf{p}} = f(c)$$

Enter an adsorption isotherm $c_{P,c}$ (SI unit: mol/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.

Concentration

Use this node to specify the species concentration on a fracture boundary (applied in points in 2D and along edges in 3D). 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 (**5**) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the COMSOL Multiphysics Reference Manual.

Flux

This node can be used to specify the species flux across a boundary of a porous fracture (applied in points in 2D and along edges in 3D). The flux of species c is defined as

$$\mathbf{n} \cdot (D_e \nabla c) = N_0$$

where N_0 is an arbitrary user-specified flux expression. For example, N_0 can represent a flux due to chemical reactions, or a phase change. A positive N_0 implies that the concentration inside the fracture increases.

INWARD FLUX

Specify the flux of each species individually. To use another boundary condition for a specific species, click to clear the check box for the mass fraction of that species.

Fracture

Use this node to model mass transport along thin fracture surfaces situated inside porous or solid material. The node assumes that the transport in the tangential direction of the fracture is dominant, as a result of lower flow resistance. Note that the fracture it self is modeled as porous.

MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the Boundary material is used.

Specify the **Porosity,** $\mathcal{E}_{\mathbf{p}}$ (dimensionless) of the porous matrix. This is by default taken From material. Select User defined to instead enter a different value.

CONVECTION

Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use The Fracture Flow Interface to compute the fluid flow velocity.

For **User defined**, enter values or expressions for the velocity components in the table shown.



The settings for the **Diffusion** is the similar to the settings for the diffusion coefficients in the Fluid node. The **Dispersion** settings are identical to the ones in the Dispersion node.

Inflow

Use this node to specify all species concentrations at a fracture inlet. The condition is applied in points in 2D and along edges in 3D.

If you want to specify the concentration of a subset of the partaking species, this can be done by using the Concentration node instead.

CONCENTRATION

For the concentration of each species $c_{0,c}$ (SI unit: mol/m³), 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: https://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 (**a**) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the COMSOL Multiphysics Reference Manual.

FURTHER READING

See the theory chapter in the section Danckwerts Inflow Boundary Condition.

No Flux

This node can be used to specify that the species flux across a boundary of a porous fracture is zero. The condition is applied in points in 2D and along edges in 3D.

Outflow

Set this condition at fracture outlets where species are transported out of the model domain by fluid motion. The condition is applied in points in 2D and along edges in 3D. It is assumed that convection is the dominating transport mechanism across outflow boundaries, and therefore that diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D_e \nabla c) = 0$$

Reactions

Use the **Reactions** node to account for the consumption or production of species through chemical reactions in the fracture. Define the rate expressions as required.

BOUNDARY SELECTION

From the **Selection** list, choose the boundaries 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 of the fracture.

REACTION RATES

Add a rate expression R_i for species i. Enter a value or expression in the field. Note that if you have the Chemistry interface available, included with the Chemical Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down menu.

REACTING VOLUME

When specifying reaction rates for a species in a fracture, the specified reaction rate may have the basis of the pore volume of the fracture, or the total volume.

- For **Total volume**, the reaction expressions in are specified per unit volume of the fracture. The reaction expressions will be multiplied by the fracture thickness d_{fr} .
- For **Pore volume**, the reaction expressions in mol/(m³·s) are specified per unit volume of total pore space in the fracture. The reaction expressions will be multiplied by the fracture thickness $d_{\rm fr}$ and the fracture porosity, $\varepsilon_{\rm p}$.

Species Source

In order to account for consumption or production of species in a fracture, the Species **Source** node adds source terms expressions S_i to the right-hand side of the species transport equations.

BOUNDARY SELECTION

From the Selection list, choose the boundaries on which to define expressions that govern the source term in the transport equations.

If there are several different parts of the fracture, with subsequent and different sources occurring within them, it might be necessary to remove some boundaries from the selection. The sources in these can then be defined using an additional Species Source node.

SPECIES SOURCE

Add a source term S_i for each of the species solved for. Enter a value or expression in the field of the corresponding species.

Theory for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution of chemical species transported by diffusion and convection. The physics interface assumes that all species present are dilute; that is, that their concentration is 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 in the Chemical Reaction Engineering Module User's Guide for more information.

Fick's law governs the diffusion of the solutes, dilute mixtures, or solutions, while the phenomenon of ionic migration is sometimes referred to as electrokinetic flow. The Transport of Diluted Species interface supports the simulations of chemical species transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D.

In this section:

- Adding Transport Through Migration
- Convective Term Formulation
- · Crosswind Diffusion
- Danckwerts Inflow Boundary Condition
- Equilibrium Reaction Theory

- Mass Balance Equation
- Mass Sources for Species Transport
- Solving a Diffusion Equation Only
- Supporting Electrolytes
- References

Note: Some features explained in this section require certain add-on modules. For details see https://www.comsol.com/products/specifications/

The section also includes the theory for The Transport of Diluted Species in Porous Media Interface:

- Adsorption
- · Convection in Porous Media
- · Diffusion in Porous Media
- Dispersion

- Mass Balance Equation for Transport of Diluted Species in Porous Media
- Mass Transport in Fractures
- Reactions

Mass Balance Equation

The default node attributed to the Transport of Diluted Species interface models chemical species transport through diffusion and convection and solves the mass conservation equation for one or more chemical species i:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i$$
 (6-2)

Equation 6-2 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/m³)
- D_i denotes the diffusion coefficient (SI unit: m²/s)
- R_i is a reaction rate expression for the species (SI unit: mol/(m³·s))
- **u** is the mass averaged velocity vector (SI unit: m/s)
- J_i is the mass flux diffusive flux vector (SI unit: mol/(m²·s))

The mass flux relative to the mass averaged velocity, \mathbf{J}_i (SI unit: mol/(m²·s)), is associated with the mass balance equation above and used in boundary conditions and flux computations. The Transport of Diluted Species interface always includes mass transport due to molecular diffusion. In this case the mass flux \mathbf{J}_i defines the diffusive flux vector

$$\mathbf{J}_i = -D\nabla c_i \tag{6-3}$$

An input field for the diffusion coefficient is available.

When Migration in Electric Fields is activated, the migration term is also added to the diffusive flux vector as shown in the section Adding Transport Through Migration.

The third term on the left side of Equation 6-2 describes the convective transport due to a velocity field **u**. This field can be expressed analytically or obtained from coupling the physics interface to one that solves for fluid flow, such as Laminar Flow. Note that all fluid flow interfaces solve for the mass averaged velocity.

On the right-hand side of the mass balance equation (Equation 6-2), R_i represents a source or sink term, typically due to a chemical reaction or desorption on a porous matrix. To specify R_i , another node must be added to the Transport of Diluted Species interface — the **Reaction** node for example, which includes an input field for specifying a reaction expression using the variable names of all participating species.

Equilibrium Reaction Theory

The feature Equilibrium Reaction is described in this section. A chemical equilibrium reaction system is defined by the stoichiometry of the reaction and the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition).

The kinetics of the reaction is so fast that the equilibrium condition is fulfilled at all times in all space coordinates.

The equilibrium condition is commonly based on the stoichiometric coefficients, v_i (dimensionless), of the reaction; the species activities of the reacting species a_i (dimensionless); and an equilibrium constant, K_{eq} (1) according to:

$$K_{\text{eq}} = \frac{\prod_{i \in \text{products}} \alpha_i^{\nu_i}}{\prod_{i \in \text{reactants}} \alpha_i^{-\nu_i}}$$

where the species activities are defined as

$$a_i = \gamma_{c,i} \frac{c_i}{c_{a0}}$$

where $c_{\rm a0}$ (SI unit: mol/m³) 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:

$$K_{\text{eq}} = \prod_{i} a_i^{\mathbf{v}_i}$$

The Equilibrium Reaction node solves for a reaction rate so that the equilibrium condition is always fulfilled in the domain. It is available for the Chemical Reaction Engineering Module; Battery Design Module; Corrosion Module; Electrochemistry Module; Electrodeposition Module; and Fuel Cell & Electrolyzer Module.



 $\gamma_{c,i}$ is set to unity when the Equilibrium constant is selected 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.

EOUILIBRIUM REACTIONS AND CONCENTRATION BOUNDARY CONDITIONS

No special treatment is made with regards to input concentration values of the Concentration boundary node. Using this feature, you can explicitly set one or a set of concentrations, and the equilibrium condition acts on the rest of the concentrations.

However, there is no solution to the problem if more concentrations than the number of species minus the number of equilibrium reactions are set using this feature.

EQUILIBRIUM REACTIONS AND TIME-DEPENDENT SIMULATIONS

Spurious oscillations may occur in a time-dependent problem if the initial conditions do not fulfill the equilibrium condition. Since equilibrium reactions are assumed to be infinitely fast, the solution is to initialize the problem using an additional study step, solving for a stationary problem with all nonequilibrium reaction rates set to zero. Manual scaling of the reaction rate dependent variables is needed in this study step.

Convective Term Formulation

The default node attributed to The Transport of Diluted Species Interface assumes chemical species transport through diffusion and convection (depending on the modules licensed, a check box to activate migration is available) and implements the mass balance equation in Equation 6-2.

There are two ways to present a mass balance where chemical species transport occurs through diffusion and convection. These are the nonconservative and conservative formulations of the convective term:

nonconservative:
$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot \mathbf{J}_i + R$$
 (6-4)

conservative:
$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}) = \nabla \cdot \mathbf{J}_i + R$$
 (6-5)

and each is treated slightly differently by the solver algorithms. In these equations \mathbf{J}_i (SI unit: mol/(m²·s)) is the diffusive flux vector, \mathbf{R} (SI unit: mol/(m³·s)) is a production or consumption rate expression, and **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 nonconservative formulation above. This is in fact the default formulation in this physics interface. To switch between the two formulations, click the **Show** button () and select **Advanced Physics Options**.

Remove the convection term from Equation 6-4 and Equation 6-5 by clearing the Convection check box in the Transport Mechanisms section for The Transport of Diluted Species Interface. The equation then becomes

$$\frac{\partial c}{\partial t} = \nabla \cdot \mathbf{J}_i + R$$

Mass Sources for Species Transport

Note: The features below are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

There are two types of mass sources in the Transport of Diluted Species interface: point sources and line sources.

POINT SOURCE

A point source is theoretically formed by assuming a mass injection/ejection, $\dot{Q}_{\rm c}$ (SI unit: mol/(m³·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_{\mathrm{p,c}}$ (SI unit: mol/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q}_{c} = \dot{q}_{p,c} \tag{6-6}$$

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 6-6, $\dot{Q}_{\rm c}$ must tend to plus or minus infinity as δV tends to zero. This means that in theory the concentration also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 6-6 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 $\dot{Q}_{\rm l,c}$ (SI unit: mol/(m³·s)), located within a tube with cross section δS and then letting δS tend to zero while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_{1,c}$ (SI unit: mol/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q}_{l,c} = \dot{q}_{l,c} \tag{6-7}$$

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

$$\dot{q}_{\mathrm{l,c}}\mathrm{test}(c)$$

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.



For feature node information, see Line Mass Source and Point Mass Source.

Note: Migration is only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

In addition to transport due to convection and diffusion, the Transport of Diluted Species interface supports ionic species transport by migration. This is done by selecting the Migration in Electric Field check box under the Transport Mechanisms section for the physics interface. The mass balance then becomes:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\text{m, }i} F c_i \nabla V + c_i \mathbf{u}) = R_i$$
 (6-8)

where

- c_i (SI unit: mol/m³) denotes the concentration of species i
- D_i (SI unit: m²/s) is the diffusion coefficient of species i
- **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
- $u_{m,i}$ (SI unit: mol·s/kg) is its ionic mobility

In this case the diffusive flux vector is

$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{\mathrm{m}, i} F c_i \nabla V$$

The velocity, **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: $J/(mol \cdot K)$) is the molar gas constant and T (SI unit: K) is the temperature.

Note: In the Nernst-Planck Equations interface, the ionic species contribute to the charge transfer in the solution. It includes an electroneutrality condition and also computes the electric potential field in the electrolyte. For more information, see Theory for the Nernst-Planck Equations Interface. This interface is included in the Chemical Reaction Engineering Module.

Supporting Electrolytes

In *electrolyte* solutions, a salt can be added to provide a high electrolyte conductivity and decrease the ohmic losses in a cell. These solutions are often called *supporting* electrolytes, buffer solutions, or carrier electrolytes. The added species, a negative and a positive ion pair, predominates over all other species. Therefore, the supporting electrolyte species can be assumed to dominate the current transport in the solution. In addition, the predominant supporting ions are usually selected so that they do not react at the electrode surfaces since the high conductivity should be kept through the process, that is, they should not be 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:

$$\mathbf{i} = F \sum_{j} -z_{j}^{2} u_{\mathrm{m},j} F c_{j} \nabla \phi \tag{6-9}$$

Equation 6-9 is simply Ohm's law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa \nabla \phi \tag{6-10}$$

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 6-10, yields:

$$\nabla \cdot (-\kappa \nabla \phi) = 0 \tag{6-11}$$

Equation 6-11 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 underresolved gradients are less smeared out.

Danckwerts Inflow Boundary Condition

Constraining the composition to fixed values at an inlet to a reactor may sometimes result in issues with unreasonably high reaction rates or singularities at the inlet boundary. These problems may many times be mitigated by using a flux boundary condition instead, based on the upstream concentrations and the fluid velocity at the boundary. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet conditions for domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an upstream concentration $c_{i,0}$, the Danckwerts inflow boundary condition prescribed the total flux as

$$\mathbf{n} \cdot (\mathbf{J}_i + \mathbf{u}c_i) = \mathbf{n} \cdot (\mathbf{u}c_{i,\,0}) \tag{6-12}$$

Mass Balance Equation for Transport of Diluted Species in Porous Media

VARIABLY SATURATED POROUS MEDIA

The following equations for the molar concentrations, c_i , describe the transport of solutes in a variably saturated porous medium for the most general case, when the pore space is primarily filled with liquid but also contain pockets or immobile gas:

$$\begin{split} \frac{\partial}{\partial t}(\theta_{l}c_{i}) + \frac{\partial}{\partial t}(\rho c_{\mathrm{P},\,i}) + \frac{\partial}{\partial t}(\theta_{\mathrm{g}}c_{\mathrm{G},\,i}) + \mathbf{u} \cdot \nabla c_{i} &= \\ \nabla \cdot \left[(D_{\mathrm{D},\,i} + D_{\mathrm{e},\,i}) \nabla c_{i} \right] + R_{i} + S_{i} \end{split} \tag{6-13}$$

On the left-hand side of Equation 6-13, 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 6-13 c_i denotes the concentration of species i in the liquid (SI unit: mol/m^3), $c_{P. i}$ the amount adsorbed to solid particles (moles per unit dry weight of the solid), and $c_{G,i}$ the concentration of species i in the gas phase.

The equation balances the mass transport throughout the porous medium using the porosity ε_p , the liquid volume fraction θ_l ; the dry bulk density, $\rho = (1 - \varepsilon_s)\rho_s$, and the solid phase density ρ_s .

For saturated porous media, the liquid volume fraction θ_l is equal to the porosity ϵ_p , but for unsaturated porous media, they are related by the saturation s as $\theta_1 = \varepsilon_p s$. The resulting gas volume fraction in the case of an unsaturated porous medium is

$$\theta_{\rm g} = \varepsilon_{\rm p} - \theta_{\rm l} = (1 - s)\varepsilon_{\rm p}$$

On the right-hand side of Equation 6-13, the first term introduces the spreading of species due to mechanical mixing resulting from the porous media (dispersion), as well as from diffusion and volatilization to the gas phase. The dispersion tensor is denoted $D_{\rm D}$ (SI unit: m²/s) and the effective diffusion by $D_{\rm e}$ (SI unit: m²/s).

The last two terms on the right-hand side of Equation 6-13 describe production or consumption of the species; R_i is a reaction rate expression which can account for reactions in the liquid, solid, or gas phase, and S_i is an arbitrary source term, for example due to a fluid flow source or sink.

Adsorption

The time evolution of the adsorption, the solute transport to or from the solid phase, is defined by assuming that the amount of solute adsorbed to the solid, $c_{P,i}$ is a function of the concentration in the fluid e_i . This implies that the solute concentration in the liquid and solid phase are in instant equilibrium. The adsorption term can be expanded to give

$$\frac{\partial}{\partial t}(\rho c_{P,i}) = \rho \frac{\partial c_{P,i}}{\partial c_i} \frac{\partial c_i}{\partial t} - c_{P,i} \rho_s \frac{\partial \varepsilon_p}{\partial t} = \rho K_{P,i} \frac{\partial c_i}{\partial t} - c_{P,i} \rho_s \frac{\partial \varepsilon_p}{\partial t}$$
(6-14)

where $K_{P,i} = \partial c_{P,i}/\partial c_i$ is the adsorption isotherm.

Volatilization

Volatilization is the process where a solute species in the liquid is transported to the gas phase due to vaporization. Assuming that the amount of solute in the gas phase, $c_{G,i}$, is a linear function of the liquid phase concentration, the volatilization term is defined as

$$\frac{\partial}{\partial t} \theta_{g} c_{G,i} = \theta_{g} \frac{\partial c_{G,i} \partial c_{i}}{\partial c_{i}} + k_{G,i} c_{i} \frac{\partial \theta}{\partial t}^{g} = \theta_{g} k_{G,i} \frac{\partial c_{i}}{\partial t} + k_{G,i} c_{i} \frac{\partial \theta}{\partial t}^{g}$$
(6-15)

where $k_{G,i} = \partial c_{G,i}/\partial c_i$ is the linear volatilization.

SATURATED POROUS MEDIA

In the case of transport in a saturated porous medium, $\theta_l = \varepsilon_p$, and the governing equations are

$$\frac{\partial}{\partial t} (\boldsymbol{\varepsilon}_{\mathbf{p}} \boldsymbol{c}_{i}) + \frac{\partial}{\partial t} (\boldsymbol{\rho} \boldsymbol{c}_{\mathbf{P},\,i}) + \mathbf{u} \cdot \nabla \boldsymbol{c}_{i} = \nabla \cdot [(\boldsymbol{D}_{\mathbf{D},\,i} + \boldsymbol{D}_{\mathbf{e},\,i}) \nabla \boldsymbol{c}_{i}] + \boldsymbol{R}_{i} + \boldsymbol{S}_{i} \tag{6-16}$$

Convection in Porous Media

Convection (also called advection) describes the movement of a species, such as a pollutant, with the bulk fluid velocity. The velocity field **u** corresponds to a superficial volume average over a unit volume of the porous medium, including both pores and matrix. This velocity is sometimes called *Darcy velocity*, and defined as volume flow

rates per unit cross section of the medium. This definition makes the velocity field continuous across the boundaries between porous regions and regions with free flow.



The velocity field to be used in the Model Inputs section on the physics interface can, for example, be prescribed using the velocity field from a Darcy's Law or a Brinkman Equations interface.

The average linear fluid velocities \mathbf{u}_{a} , provides an estimate of the fluid velocity within the pores:

$$\mathbf{u}_{\mathrm{a}} = \frac{\mathbf{u}}{\varepsilon_{\mathrm{p}}}$$
 Saturated $\mathbf{u}_{\mathrm{a}} = \frac{\mathbf{u}}{\theta_{\mathrm{l}}}$ Unsaturated

$$\mathbf{u}_{a} = \frac{\mathbf{u}}{\theta_{1}}$$
 Unsaturated

where ε_p is the porosity and θ_l = $s\varepsilon_p$ the liquid volume fraction, and s the saturation, a dimensionless number between 0 and 1.



Figure 6-2: 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 6-13 is written as:

$$\begin{split} \frac{\partial}{\partial t}(\boldsymbol{\theta}_{l}\boldsymbol{c}_{i}) + \frac{\partial}{\partial t}(\boldsymbol{\rho}\boldsymbol{c}_{\mathrm{P},\,i}) + \frac{\partial}{\partial t}(\boldsymbol{\theta}_{g}\boldsymbol{c}_{\mathrm{G},\,i}) + \nabla \cdot \mathbf{u}\boldsymbol{c}_{i} &= \\ \nabla \cdot \left[(\boldsymbol{D}_{\mathrm{D},\,i} + \boldsymbol{D}_{\mathrm{e},\,i}) \nabla \boldsymbol{c}_{i} \right] + \boldsymbol{R}_{i} + \boldsymbol{S}_{i} \end{split} \tag{6-17}$$

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c_i \nabla \cdot \mathbf{u}$, would equal zero for an incompressible fluid and would result in the nonconservative formulation described in Equation 6-13.

When using the nonconservative formulation, which is the default, the fluid is assumed incompressible and divergence free: $\nabla \cdot \mathbf{u} = 0$. The nonconservative formulation improves the stability of systems coupled to a momentum equation (fluid flow equation).



To switch between the two formulations, click the **Show** button (**5**) and select Advanced Physics Options. In the section Advanced Settings select either Nonconservative 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, $D_{\rm e}$, depends on the structure of the porous material and the phases involved. Dependent on whether the transport of diluted species occurs in free flow, saturated or unsaturated porous media, the effective diffusivity is defined as:

$$\begin{split} D_{\rm e} &= D_F & \text{Free Flow} \\ D_{\rm e} &= \frac{\varepsilon_{\rm p}}{\tau_L} D_L & \text{Saturated Porous Media} \\ D_{\rm e} &= \frac{\theta_{\rm l}}{\tau_{\rm L}} D_{\rm L} & \text{Unsaturated Porous Media} \\ D_{\rm e} &= \frac{\theta_{\rm l}}{\tau_{\rm L}} D_{\rm L} + \frac{\theta_{\rm g}}{\tau_{\rm G}} k_{\rm G} D_{\rm G} & \text{Unsaturated with Volatilization} \end{split}$$

Here $D_{
m F},D_{
m L}$, and $D_{
m G}$ are the single-phase diffusion coefficients for the species diluted in a fluid, a pure liquid, and a gas phase, respectively (SI unit: m^2/s), and τ_F , τ_I , and τ_{G} are the corresponding tortuosity factors (dimensionless).

The tortuosity factor accounts for the reduced diffusivity due to the fact that the solid grains impede Brownian motion. The interface provides predefined expressions to

compute the tortuosity factors in partially saturated porous media according to the Millington and Quirk model (Ref. 12):

$$\tau_L = \theta_l^{-7/3} \varepsilon_p^2, \ \tau_G = \theta_g^{-7/3} \varepsilon_p^2$$

and Bruggeman model

$$\tau_L = \theta_l^{-5/2} \varepsilon_p^2$$
, $\tau_G = \theta_g^{-5/2} \varepsilon_p^2$

For saturated porous media $\theta_l = \epsilon_p$. The fluid tortuosity for the Millington and Quirk model is

$$\tau_L = \varepsilon_p^{-1/3}$$

and for the Bruggeman model the tortuosity is defined as

$$\tau_L = \varepsilon_p^{-1/2}$$

User defined expressions for the tortuosity factor can also be applied.

Dispersion

The contribution of dispersion to the mixing of species typically overshadows the contribution from molecular diffusion, except when the fluid velocity is very small.

The spreading of mass, as a fluid travel through a porous medium is caused by several contributing effects. Local variations in fluid velocity lead to mechanical mixing referred to as dispersion occurs because the fluid in the pore space flows around solid particles, so the velocity field varies within pore channels. The spreading in the direction parallel to the flow, or longitudinal dispersivity, typically exceeds the transverse dispersivity from up to an order of magnitude. Being driven by the concentration gradient alone, molecular diffusion is small relative to the mechanical dispersion, except at very low fluid velocities.

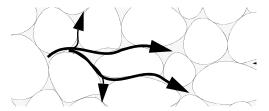


Figure 6-3: Spreading of fluid around solid particles in a porous medium.

The dispersion is controlled through the dispersion tensor D_D . The tensor components can either be given by user-defined values or expressions or derived from the directional dispersivities.

Using the longitudinal and transverse dispersivities in 2D, the dispersivity tensor components are (Ref. 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_{Dii} (SI unit: m²/s) are the principal components of the dispersivity tensor, and $D_{{
m D}ji}$ and $D_{{
m D}ji}$ are the cross terms. The parameters $lpha_{
m L}$ and $lpha_{
m T}$ (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:

$$\begin{split} D_{Lxx} &= \alpha_{1} \frac{u^{2}}{|\mathbf{u}|} + \alpha_{2} \frac{v^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{w^{2}}{|\mathbf{u}|} \\ D_{Lyy} &= \alpha_{1} \frac{v^{2}}{|\mathbf{u}|} + \alpha_{2} \frac{u^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{w^{2}}{|\mathbf{u}|} \\ D_{Lzz} &= \alpha_{1} \frac{w^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{u^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{v^{2}}{|\mathbf{u}|} \\ D_{Lxy} &= D_{Lyx} = (\alpha_{1} - \alpha_{2}) \frac{uv}{|\mathbf{u}|} \\ D_{Lxz} &= D_{Lzx} = (\alpha_{1} - \alpha_{3}) \frac{uw}{|\mathbf{u}|} \\ D_{Lyz} &= D_{Lzy} = (\alpha_{1} - \alpha_{3}) \frac{vw}{|\mathbf{u}|} \end{split}$$

In Equation 6-18 the fluid velocities u, v, and w correspond to the components of the velocity field \mathbf{u} in the x, y, and z directions, respectively, and α_1 (SI unit: m) is the longitudinal dispersivity. If z is the vertical axis, α_2 and α_3 are the dispersivities in the transverse horizontal and transverse vertical directions, respectively (SI unit: m). Setting $\alpha_2 = \alpha_3$ gives the expressions for isotropic media shown in Bear (Ref. 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 four predefined and one user defined relationships to predict the solid concentrations, e_{Pi} from the concentration in the liquid phase, e_i :

$$c_{\rm P} = c_{\rm Pmax} \frac{K_{\rm L}c}{1 + K_{\rm L}c} \qquad \text{Langmuir}$$

$$c_{\rm P} = K_{\rm F} \left(\frac{c}{c_{\rm ref}}\right)^{N} \qquad \text{Freundlich}$$

$$c_{\rm P} = c_{\rm Pmax} \frac{b_{\rm T}c}{\left(1 + \left(b_{\rm T}c\right)^{N_{\rm T}}\right)^{1/N_{\rm T}}} \qquad \text{Toth}$$

$$c_{\rm P} = \frac{K_{\rm B}c_{\rm 0}c}{\left(c_{\rm S} - c\right)\left(1 + \left(K_{\rm B} - 1\right)\frac{c}{c_{\rm S}}\right)} \qquad \text{BET}$$

The above equations contains the following parameters:

- Freundlich: Freundlich constant $K_{\rm F}$ (SI unit: mol/kg), Freundlich exponent $N_{\rm F}$ (dimensionless), and reference concentration c_{ref} (SI unit: mol/m³).
- Langmuir: Langmuir constant $K_{\rm L}$ (SI unit: m³/mol), and adsorption maximum c_{Pmax} (SI unit: mol/kg).
- Toth: Toth constant b_T (SI unit: m³/mol), Toth exponent N_T (dimensionless), and adsorption maximum c_{Pmax} (SI unit: mol/kg).
- BET (Braunauer-Emmett-Teller): BET constant $K_{\rm B}$ (dimensionless), and a monolayer adsorption capacity c_0 (SI unit: mol/kg) and a Saturation concentration, $c_{\rm S}({\rm SI~unit:~mol/m}^3)$.

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, nonequilibrium 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}_c relative to the average linear velocity of the fluid, \mathbf{u}_{a} , as in

$$RF = 1 + \frac{\rho_b}{\theta} \frac{\partial c_P}{\partial c} = \frac{\mathbf{u}_a}{\mathbf{u}_c}$$

If the contaminant moves at the average linear velocity of the fluid for RF = 1. For RF > 1, the contaminant velocity is smaller than the fluid velocity owing to residence time on solids.

Chemical reactions of all types influence species transport in porous media. Examples include biodegradation, radioactive decay, transformation to tracked products, temperature- and pressure-dependent functions, exothermic reactions, and endothermic reactions. The reactions represent change in species concentration per unit volume porous medium per time. Reaction terms are used on the right-hand side of the governing equation to represent these processes. For reactions in a fluid phase, multiply the expression by the fluid volume fraction θ . Similarly, solid phase reaction expressions include the bulk density, ρ_b , and gas phase reactions include the gas volume fraction, $a_{\rm v}$.

The following expressions define some common types of reactions:

$$\begin{split} R_{Li} &= -\theta \frac{\ln 2}{\lambda_{Li}} c_i & \text{Radioactive decay} - \text{liquid} \\ R_{Pi} &= -\rho_{\text{b}} \frac{\ln 2}{\lambda_{Pi}} \Big(\frac{\partial c_{Pi}}{\partial c_i} \Big) c_i \text{Radioactive decay} - \text{solid} \\ R_{Gi} &= -\frac{\ln 2}{\lambda_{Gi}} a_{\text{v}} \Big(\frac{\partial c_{Gi}}{\partial c} \Big) c_i \text{Radioactive decay} - \text{gas} \\ R_{Lk} &= \theta \zeta_{Li} c_i & \text{Creation from parent } c_{Li} - \text{liquid} \\ R_{Pk} &= \rho_{\text{b}} \zeta_{Pi} \Big(\frac{\partial c_{Pi}}{\partial c_i} \Big) c_i & \text{Creation from sorbed parent } c_{Pi} - \text{solid} \\ R_{Gk} &= -\zeta a_{\text{v}} \Big(\frac{\partial c_{Gi}}{\partial c} \Big) c_i & \text{Reaction} - \text{gas} \end{split}$$

where λ is the chemical half life, ζ is a reaction rate, and the subscripts L, P, and G denote liquid, solid, and gas phases, respectively. In the equations, the reactions either depend on liquid concentration c_i or solid phase concentrations c_{Pi} obtained using the sorption derivative with c_i or gas phase concentration c_{Gi} depending on the gas volume fraction, the volatilization, and the liquid concentration.

Reaction rates can vary with results from other equations in your model, such as temperature. For example, enter the Arrhenius rate law given in Ref. 13:

$$\zeta_T = \zeta_R \exp\left[\frac{E_a(T - T_R)}{R_u T T_R}\right]$$
 (6-20)

In Equation 6-20, T denotes the current absolute temperature, T_R denotes the reference absolute temperature, E_a is the activation energy, and R_u is the universal gas constant.

Mass Transport in Fractures

When thin fractures occur in porous media, fluid flow tends to move faster along the fracture than in the surrounding media. The transport of chemical species therefore also occur also faster in the direction of the fractures.

The fluid flow in a fracture can be modeled using Darcy's law formulated in a thin sheet of porous medium (a fracture):

$$\mathbf{u} = \frac{\kappa}{\mu} \nabla_{\mathbf{t}} p$$

Here **u** is the tangential Darcy velocity, κ is the fracture permeability, μ the fluid's dynamic viscosity, and $\nabla_t p$ is the tangential gradient of the fluid pressure.

The equation to solve for mass transport of species e_i in a thin fracture, embedded in a porous media, is derived from Equation 6-13. The resulting equation is:

$$d_{\text{fr}} \left(\frac{\partial \rho_{\text{b}} c_{\text{P},i}}{\partial t} + \frac{\partial \varepsilon_{\text{p}} c_{i}}{\partial t} + \nabla_{\text{t}} \cdot (D_{\text{e},i} \nabla_{\text{t}} c_{i}) + \mathbf{u} \cdot \nabla_{\text{t}} c_{i} \right) = d_{\text{fr}} R_{i} + d_{\text{fr}} S_{i} + n_{0} \quad (6\text{-}21)$$

Here $d_{\rm fr}$ is the fracture thickness, $c_{\rm P, \it i}$ the amount of species adsorbed to (or desorbed from) the porous matrix (moles per unit dry weight of the solid), $\varepsilon_{\rm p}$ is the fracture porosity, and $D_{\rm e}$ is the effective diffusivity. The first two terms on the right hand side represent source terms from reactions, and n_0 corresponds to out-of plane flux from the adjacent porous domain.

In order to arrive at the tangential differential equation, the gradient is split into the contributions normal and tangential to the fracture:

$$\nabla c_i = \nabla_{\mathbf{n}} c_i + \nabla_{\mathbf{t}} c_i$$

The normal gradient is defined in the direction normal to the boundary representing the fracture and the tangential gradient is defined along the boundary. Assuming that the variations in the normal (thin) direction of the fracture are negligible compared to those in the tangential direction, the gradient is simplified as:

$$\nabla c_i = \nabla_{\mathbf{t}} c_i$$

Using The Transport of Diluted Species in Fractures Interface, the transport along fracture boundaries alone is solved for. In this case the transport in the surrounding porous media neglected and the out-of plane flux n_0 vanishes.



See Fracture for more information about the boundary feature solving Equation 6-21. See The Transport of Diluted Species in Fractures Interface for more information about the physics interface solving the equation on boundaries only.

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Heat Transfer Interfaces

This chapter has information about the heat transfer interfaces used for modeling, particularly in porous media. As with all other physical descriptions simulated by COMSOL Multiphysics $^{\circledR}$, any description of heat transfer can be directly coupled to any other physical process. This is particularly relevant for systems based on chemical reactions and mass transfer along with fluid flow. These physics interfaces are found under the **Heat Transfer** branch () when adding a physics interface.

In this chapter:

• The Mechanisms for Heat Transfer

The documentation of all features in the Heat Transfer and Heat Transfer in Porous Media interfaces are available in the *Heat Transfer Module User's Guide*, specifically in these sections:

- The Heat Transfer Module Interfaces
- The Heat Transfer in Porous Media Interface
- The Heat Transfer in Fractures Interface
- Theory for the Heat Transfer Module
- Theory for Heat Transfer in Porous Media
- Theory for Heat Transfer in Thin Structures

The Mechanisms for Heat Transfer

This section includes these topics:

- Selecting the Right Heat Transfer Interface
- · Heat Conduction
- Heat Convection and Conduction
 - The Heat Transfer Module Interfaces
 - Theory for the Heat Transfer Module



- The Heat Transfer in Porous Media Interface
- Theory for Heat Transfer in Porous Media
- The Heat Transfer in Fractures Interface
- Theory for Heat Transfer in Thin Structures

Selecting the Right Heat Transfer Interface

The Heat Transfer branch included with the Subsurface Flow Module license includes a number of subbranches to describe energy transport.

Heat transfer through conduction and convection (both nonisothermal flow and conjugate heat transfer) in solid and free media is supported by physics interfaces shipped with the basic COMSOL Multiphysics license.

If you are using this module with enhanced Heat Transfer interface features, see also the Heat Transfer Module documentation for additional information. See Where Do I Access the Documentation and Application Libraries?

This module also includes The Heat Transfer in Porous Media Interface. The physics interface itself supports heat transfer in porous media where the thermal conductivity and heat capacity are affected by the extent of porosity. As a porous media is made up of a solid matrix filled with a fluid, heat is transported at different rates through the two types of media. The Heat Transfer in Porous Media interface provides tools and support for defining an appropriate matrix model.

The Heat Transfer in Porous Media interface characterizes temperature distributions for geological phenomena and freely couple to other features in a model. The physics interface applies to systems consisting of porous media, solids and fluids. Included are physics interfaces to calculate effective properties for porous media consisting of fluids and solid components, or a rock formation with different mineral proportions. The physics interface also features predefined expressions to represent the geotherm as a radiogenic heat source.

The Heat Transfer in Fractures (htlsh) interface ((1)), found in the Thin Structures physics area under the **Heat Transfer** branch (), is used to model heat transfer by conduction and convection in layered materials represented by boundaries. The interface is active on all boundaries where a layered material is defined, with a Porous **Medium** model active by default. All functionalities for including other boundary contributions, such as surface-to-ambient radiation, are also available.

Heat Conduction

The Heat Transfer interface in this module provides tools for analyzing heat transfer that is proportional to a temperature gradient, or conduction. It accounts explicitly for the geotherm as a heat source. This physics interface provides options to calculate thermal properties for multicomponent media. It incorporates boundary and source options to represent transversal fluxes such as convection and radiation at adjacent domains that you do not explicitly model.

The physics interface describes heat flow with negligible impacts of moving fluids. Just a few targets for conduction modeling include resistive heating in cores, estimating a surface heat flux, describing a temperature profile with depth, phase changes, exothermic reactions, and cooling earth analyses. The physics interface provides tools to consider radiative and convection heat transfers at boundaries so that you can focus on the physics in the domain of interest. With the COMSOL Multiphysics "just-type-it-in" modeling flexibility, it is straightforward to create nonlinear expressions where, for example, thermal conductivity varies with temperature as well as other physics.

Heat conduction figures into radiogenic decay, pressure-temperature phase changes, cooling-earth models, radiation, exothermic and endothermic reactions of solutes, microbial processes, diurnal heating, and many other earth processes. Conductive heat transfer can be long-term steady or exquisitely sensitive over tiny time increments. It can involve molten materials, mineral grains, fluids trapped within interstices, human-made structures, and molten rock. The heat conduction can operate within closed systems, but the geometry of interest often interacts at edges and surfaces with adjacent domains through moving fluids, conduction across a semi-insulating layer,

and radiation. The models can cover such large distances that the tiny amount of heat given off by the spontaneous decay of the radiogenic particles present in most rocks produces the discernible temperature gradient with depth known to many as the geotherm.

Heat Convection and Conduction

The Heat Transfer in Porous Media Interface can also set up analyses for heat transferred by convection and conduction for subsurface flow applications. Use this physics interface to describe heat carried by moving oil, water, or magma that you describe with a velocity field. Presumably the fluid velocity is nonzero but not necessarily so. You can couple the Heat Transfer interface to a Fluid Flow interface if you want to model, for example, rising magma, hot springs, liquid-steam transfers, conduction in a solid rock, buoyancy flow in streams, magma convection, and hot oil moving through a pipe. For models involving large depth changes, this physics interface provides a number of options to characterize the geothermal gradient.

The physics interface assumes that the model domain includes a single fluid moving through a domain with a number of immobile constituents, including several different solids and trapped fluids. Such is the case in many porous media.

The physics interface can also describe heat transferred with a moving fluid, which can be a surface flow or one confined to interstices in a porous medium. Analyses can cover thermal pollution migrating in a stream, transfer of hot oil into and up a well, steam injection, and diurnal heating in variably saturated soil.

In this context it is worth mentioning that it is possible to model inflow of heat through a virtual domain at inlet boundaries of fluid domains using the so-called Inflow boundary condition. Accordingly, an Outflow Boundary condition is available at the outlet. Furthermore, an Open Boundary condition is available to define a boundary as the limit between a non-solid domain of the geometry and the rest of the same fluid domain that is not represented in the geometry. At the open boundary both inflow and outflow conditions are supported.

This physics interface easily combines with others for an unlimited number of interesting analyses. Consider, for example, that it is straightforward to include the impacts of temperature change on hydraulic conductivity, biodegradation and chemical reaction rates, electric and magnetic potential fields, and rock strength. Likewise, you can feed back results of other physics, including reactions that consume heat, to a heat transfer model.

Phase Change

When modeling heat transfer in solids, fluids, and porous media, the properties of a phase changing material are specified according to the apparent heat capacity formulation. This formulation gets its name from the fact that the latent heat is included as an additional term in the heat capacity.

The subnode **Phase Change Material** is available under the Solid, Fluid, or Porous Medium node.

With phase transitions in porous media, there is often a remaining phase that does not participate in the phase transition. For example, water in the soil, which does not freeze even at values far lower than 0 degrees, or water in food, which does not evaporate completely during cooking. To consider such residual phases Immobile Fluids (Porous Medium) can be used.



Frozen Inclusion: Application Library path

Subsurface_Flow_Module/Heat_Transfer/frozen_inclusion

A more detailed description of the functionalities mentioned above and the discussion of a variety of modeling techniques can be found in the following sections of the Heat Transfer Module User's Guide:

- Heat Transfer Variables
- Using the Boundary Conditions for the Heat Transfer Interfaces
- Handling Frames in Heat Transfer
- Heat Transfer Consistent and Inconsistent Stabilization Methods
- Heat Transfer and Fluid Flow Coupling
- Solver Settings
- Theory for the Inflow Boundary Condition
- Theory for Heat Transfer with Phase Change

See also The Heat Transfer Module Interfaces and Theory for the Heat Transfer Module.

Multiphysics Interfaces and Couplings

The Subsurface Flow Module contains predefined multiphysics interfaces for poroelasticity and multiphase flow in porous media. When a predefined multiphysics interface is added from the **Model Wizard** or **Add Physics** window, it adds the constituent interfaces and the **Multiphysics** node which automatically includes one or more multiphysics couplings.

In this chapter:

- Theory for the Poroelasticity Interfaces
- The Poroelasticity Interfaces
- Theory for the Multiphase Flow in Porous Media Interface
- The Multiphase Flow in Porous Media Interface
- The Reacting Flow in Porous Media Interface
- The Nonisothermal Flow, Brinkman Equations Interface

Theory for the Poroelasticity Interfaces

Small Strain Poroelasticity

Poroelasticity theory describes the interaction between fluid flow and deformation in elastic porous media. This bidirectional multiphysics coupling relates fluid flow and solid deformation with linear constitutive relations.

Of the two constitutive relations governing poroelastic behavior, one relates the stress, strain, and pore pressure:

$$\sigma = \mathbf{C} : \varepsilon - \alpha_{\mathbf{R}} p_{f} \mathbf{I} \tag{8-1}$$

Here, σ is the Cauchy stress tensor, ϵ is the strain tensor, α_B is the *Biot–Willis* coefficient, and p_f is the fluid pore pressure. For linear elasticity, the coefficients in the elasticity matrix C must be measured under "drained" conditions, by measuring the strain induced by a change in stress (or by measuring the induced stress by changes in strain) under constant pore pressure.

By splitting the above relation into volumetric and a deviatoric parts, it can be seen that the deviatoric part (shear stress) is independent of the pore pressure. For an isotropic linear elastic material, this means that

$$dev(\sigma) = 2G_d dev(\varepsilon)$$

where G_d is the shear modulus of the drained porous matrix.

The volumetric coupling is derived by taking the trace of Equation 8-1

$$-p_{\rm m} = K_{\rm d} \varepsilon_{\rm vol} - \alpha_{\rm R} p_{\rm f}$$

where the mean pressure (positive in compression) is calculated from the trace of the stress tensor σ as $p_{\rm m}$ = -trace(σ)/3 . $K_{\rm d}$ is the bulk modulus of the drained porous matrix, and the volumetric strain ε_{vol} is a measurement of the porous matrix dilation or contraction (negative in compression).

Note that the **Poroelasticity** multiphysics coupling adds the contribution from the pore pressure, p_{f} , as a load. In this setting, the stress tensor σ and mean pressure p_{m} are effective stress measures.



The mean pressure is available from the Solid Mechanics interface in the variable solid.pm and the volumetric strain in the variable solid.evol. The fluid pore pressure is available from the Darcy's Law interface in the dependent variable p.

The other constitutive relation in Biot's theory of poroelasticity (Ref. 1) relates the increment in fluid content ζ to changes in volumetric strain and pore pressure. The pore pressure is proportional to the dilation of the porous matrix and the variation of fluid content:

$$p_{\rm f} = M(\zeta - \alpha_{\rm R} \varepsilon_{\rm vol}) \tag{8-2}$$

Biot and Willis (Ref. 1) measured the coefficients $\alpha_{\rm B}$ and M with the unjacketed compressibility test and derived expressions for these coefficients in terms of solid and fluid bulk moduli (or compressibilities).

The variable M, sometimes called the Biot modulus, is the inverse of the storage coefficient S_p in Darcy's law. It is defined through Equation 8-2 as the change in fluid content due to changes in pore pressure under constant deformation (constant volumetric strain):

$$S_{\rm p} = \frac{1}{M} = \frac{\partial \zeta}{\partial p_{\rm f}} \Big|_{\varepsilon_{ii}}$$

Using this definition, it is possible to measure the storage coefficient S_p directly in the lab, and, in the case of an ideal isotropic porous material, it can be calculated from basic material properties as

$$S_{\rm p} = \frac{\varepsilon_{\rm p}}{K_{\rm f}} + \frac{\alpha_{\rm B} - \varepsilon_{\rm p}}{K_{\rm s}} \tag{8-3}$$

where $\varepsilon_{\rm p}$ is the porosity, $K_{\rm f}$ the fluid bulk modulus (the inverse of the fluid compressibility χ_f), and K_s the solid bulk modulus; that is, the theoretical bulk modulus of a homogeneous block of the solid material making up the porous matrix.

The Biot-Willis coefficient, $\alpha_{\rm B}$, relates the volume of fluid expelled (or sucked into) a porous material element due to the volumetric change of the same element. This

coefficient can be measured experimentally as the change of mean pressure due to changes in the pore pressure under constant deformation (constant volumetric strain). In the case of an ideal isotropic porous material it can be defined in terms of the drained and solid bulk moduli as

$$\alpha_{\rm B} = \frac{\partial p_{\rm m}}{\partial p_{\rm f}} \bigg|_{\epsilon_{\rm ii}} = 1 - \frac{K_{\rm d}}{K_{\rm s}}$$

The drained bulk modulus $K_{\rm d}$ is always smaller than the solid bulk modulus $K_{\rm s}$ (a solid block is stiffer than a porous block made of the same material), and therefore the Biot-Willis coefficient is bounded to $\varepsilon_p \le \alpha_B \le 1$.

The parameter α_B does not depend on the properties of the fluid, but on the properties of the porous matrix. A soft porous matrix is represented by a Biot-Willis coefficient close to unit (since $K_d << K_s$), while for a stiff matrix, α_B is close to the porosity ε_p , since $K_d \approx (1 - \varepsilon_p) K_s$.

By replacing $K_s = (1 - \alpha_B)/K_d$, the storage coefficient S_p in Equation 8-3 is calculated in terms of the porosity ε_p , the Biot-Willis coefficient α_B , and the bulk moduli of the fluid K_f and the drained porous matrix K_d as

$$S_{p} = \frac{\varepsilon_{p}}{K_{f}} + (\alpha_{B} - \varepsilon_{p}) \frac{(1 - \alpha_{B})}{K_{d}}$$
(8-4)

For a soft porous matrix, $\alpha_B\approx 1$, or for a stiff porous matrix, $\alpha_B\approx \epsilon_p$, the lower bound for the poroelastic storage is $S_p \approx \varepsilon_p / K_f$.

The linear momentum balance for a fully-saturated porous solid in equilibrium under gravitational load reads

$$-\nabla \cdot \boldsymbol{\sigma} = -\nabla (\alpha_{\rm B} p_{\rm f}) + \rho_{\rm av} \mathbf{g} \tag{8-5}$$

where σ is the stress tensor computed from linear elasticity, and \mathbf{g} is the gravitational acceleration,. The average density ρ_{av} is computed from

$$\rho_{\rm av} = \rho_{\rm f} \varepsilon_{\rm p} + \rho_{\rm d}$$

where ρ_f represents the fluid density and ρ_d the density of the dry porous matrix.

The fluid-to-structure coupling enters as an additional volumetric force in the momentum equation as described in Equation 8-5, which can be identified as an external load due to the fluid pressure, see External Stress in the Structural Mechanics Module User's Guide for details.

Equation 8-5, which describes an equilibrium state (inertial effects are neglected), also applies to the case of a time-dependent flow model. This is a valid assumption in geotechnical applications since the time scale of the structural response is generally many orders of magnitude faster than the time scale of the flow. When you study the coupled process on the time scale of the flow, you can therefore assume that the solid reaches a new equilibrium immediately in response to a change in the flow conditions. This means that the stresses and strains change in time – even if Equation 8-5 appears to be stationary – and that the structure-to-fluid coupling term, involving the rate of strain, is nonzero.

When **Include inertial terms** is selected, the average density is used in the inertial term for the momentum equation. In the presence of a volume force \mathbf{f} (e.g. gravity), the momentum balance then reads

$$\rho_{\text{av}} \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \mathbf{\sigma} = -\nabla (\alpha_{\text{B}} p_{\text{f}}) + \mathbf{f}$$
 (8-6)

where **u** represents the solid displacement and ρ_{av} the average density.

Inertial effects are also included when modeling waves in saturated porous media, see the Theory for the Poroelastic Waves Interfaces section in the Acoustics Module User's Guide for details.

Darcy's Law

Darcy's law describes the flow field in the poroelastic medium. The fluid equation comes from the mass conservation

$$\frac{\partial}{\partial t}(\rho_{\rm f}\varepsilon_{\rm p}) + \nabla \cdot (\rho_{\rm f}\mathbf{v}) = Q_{\rm m} \tag{8-7}$$

where ho_f is the fluid density, ho_p is the porosity, and Q_m is a mass sink or source. The fluid velocity is computed from Darcy's law

$$\mathbf{v} = -\frac{\kappa}{\mu} \nabla p_{\mathbf{f}}.$$

where κ is the permeability of the porous matrix, μ is the fluid viscosity, and p_f is the fluid pressure in the pores. If gravity is included, Darcy's velocity is augmented by

$$\mathbf{v} = -\frac{\kappa}{\mu} (\nabla p_{\rm f} + \rho_{\rm f} \mathbf{g})$$

where **g** is the gravitational acceleration. Note that the fluid velocity is actually the relative velocity of the fluid with respect to the pore walls.

The storage model S_p for linear poroelasticity is derived from

$$\frac{\partial}{\partial t}(\rho_{f}\varepsilon_{p}) = \rho_{f}S_{p}\frac{\partial p_{f}}{\partial t}$$

where the poroelastic storage term S_p is calculated from Equation 8-4.

For small strain poroelasticity, the mass source or sink $Q_{
m m}$ reads

$$Q_{\rm m} = -\rho_{\rm f} \alpha_{\rm B} \frac{\partial}{\partial t} \varepsilon_{\rm vol}$$

where $\partial \varepsilon_{\text{vol}}/\partial t$ is the rate of change in volumetric strain (of the porous matrix), ρ_f is the fluid density, and α_B is the Biot-Willis coefficient. You can interpret the right-hand-side term as the rate of expansion of the pore space. As ε_{vol} increases with time, the volume fraction available for the fluid increases and thereby gives rise to a fluid sink; as indicated by the negative sign in the source term $Q_{\rm m}$.

The poroelastic storage, together with the expression for the mass source, and the definition of Darcy's velocity translate the mass conservation equation, Equation 8-7, into

$$\rho_{\rm f} S_{\rm p} \frac{\partial p_{\rm f}}{\partial t} + \nabla \cdot (\rho_{\rm f} \mathbf{v}) = -\rho_{\rm f} \alpha_{\rm B} \frac{\partial}{\partial t} \varepsilon_{\rm vol}$$
 (8-8)

Large Strain Poroelasticity

When a porous body experiences large deformations (large strains or large rotations), the infinitesimal theory cannot be used. In a large deformation context, the momentum equation, Equation 8-6, reads

$$\rho_{\text{av}} \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot P^T = \mathbf{f} \tag{8-9}$$

where the gradient $\nabla = \partial / \partial \mathbf{X}$ corresponds to the material gradient with respect to the undeformed configuration, and P is the nominal (first Piola-Kirchoff) stress tensor. See Equation of Motion in the Structural Mechanics Theory chapter for details.

The pore pressure contribution enters as a load in Equation 8-9. The first Piola-Kirchoff load generated from the pore pressure reads

$$P_{\rm p} = \alpha_{\rm R} p_{\rm f} J F^{-T} \tag{8-10}$$

Darcy's law is also written with respect to the undeformed configuration. Darcy's velocity in the undeformed configuration reads

$$\mathbf{V} = -\frac{\kappa}{\mu} \nabla p_{\mathrm{f}}$$

where, κ is the permeability of the undeformed porous matrix, μ is the fluid viscosity, and p_f is the fluid pressure in the pores. The symbol $\nabla = \partial/\partial \mathbf{X}$ corresponds to the gradient with respect to the undeformed configuration.

Darcy's velocity in the current (deformed) configuration is then computed with the so-called *Piola transformation* (Ref. 2)

$$\mathbf{v} = \frac{1}{J} F \cdot \mathbf{V}$$

where F is the deformation gradient, and J the volume change.

The mass conservation, Equation 8-8, is then written as (Ref. 2)

$$\rho_{\rm f} S_{\rm p} \frac{\partial p_{\rm f}}{\partial t} + \frac{1}{J} \nabla \cdot (\rho_{\rm f} \mathbf{V}) = -\rho_{\rm f} \alpha_{\rm B} \frac{\partial}{\partial t} \varepsilon_{\rm vol} \tag{8-11}$$

where the rate of volumetric strain is now computed from Hencky's strain

$$\frac{\partial}{\partial t} \varepsilon_{\text{vol}} = \frac{\partial}{\partial t} \log J = \frac{1}{J} \frac{\partial J}{\partial t}$$

For large strain poroelasticity, the poroelastic storage is computed from the current porosity, and not from the porosity of the undeformed porous matrix. The porosity of the deformed porous matrix, ϕ , is related to the porosity of the undeformed material $\varepsilon_{\rm p}$ as

$$\phi = \frac{1}{J} \varepsilon_{\rm p}$$

so the poroelastic storage (Equation 8-3) in a large strain context reads

$$S_{\rm p} = \frac{\phi}{K_c} + \frac{\alpha_{\rm B} - \phi}{K_c} \tag{8-12}$$

For numerical reasons, and also since the solid mechanics equations are solved in a total Lagrangian formulation (see Lagrangian Formulation for details), it is more efficient to write the mass conservation equation for the fluid in the undeformed configuration. This is done by multiplying Equation 8-11 by the volume change J, so it reads

$$\rho_{\rm f} S_{\rm p} J \frac{\partial p_{\rm f}}{\partial t} + \nabla \cdot (\rho_{\rm f} \mathbf{V}) = -\rho_{\rm f} \alpha_{\rm B} \frac{\partial J}{\partial t} \tag{8-13}$$

In order to track large deformations in the porous matrix, the Poroelasticity, Large Deformations multiphysics interface also adds an Elastic Predeformation node to the Solid Mechanics interface. See Elastic Predeformation for details.

Reference for the Poroelasticity Interface

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- 2. O. Coussy. Poromechanics. John Wiley & Sons, 2004.

The Poroelasticity Interfaces

The Poroelasticity, Solid Interface

The **Poroelasticity, Solid** interface (**N**) combines a transient formulation of Darcy's law with a quasistatic formulation of Solid Mechanics. The coupling occurs on the domain level, where the pore pressure from the Darcy's Law interface acts as a load for the Solid Mechanics interface, causing swelling or shrinking. Changes in volumetric strain affect the pore space, acting as a mass source or sink in Darcy's Law.

When a predefined **Poroelasticity**, **Solid** interface is added from the **Structural Mechanics** branch () of the Model Wizard or Add Physics windows, Solid Mechanics and Darcy's **Law** interfaces are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the **Poroelasticity** multiphysics coupling.

On the Constituent Physics Interfaces

- The Solid Mechanics interface is described in the The Solid Mechanics Interface.
- The Darcy's Law interface is described in The Darcy's Law Interface.



To model orthotropic or anisotropic porous materials requires the Structural Mechanics Module. For information about the constitutive equations and theory background, see Structural Mechanics Theory.



Theory for the Poroelasticity Interfaces.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Poroelasticity**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single Solid Mechanics and Darcy's Law interfaces are added, an empty **Multiphysics** node appears in the model tree. You can choose from the available coupling features, but the settings in the constituent interfaces are not modified.



Coupling features are available from the context menu (right-click the **Multiphysics** node) or from the **Physics** toolbar, **Multiphysics** menu.

TABLE 8-1: MODIFIED SETTINGS FOR A POROELASTICITY INTERFACE

PHYSICS INTERFACE OR COUPLING FEATURE	MODIFIED SETTINGS
Solid Mechanics	For the Solid Mechanics interface, under Structural Transient Behavior the Structural transient behavior is set to Quasistatic.
Darcy's Law	For the Darcy's Law interface, a Poroelastic storage model is added by default.
Poroelasticity	The Domain Selection is the same as that of the participating physics interfaces. The corresponding Solid Mechanics and Darcy's Law interfaces are preselected in the Coupled Interfaces section.



Failure of a Multilateral Well: Application Library path Subsurface_Flow_Module/Flow_and_Solid_Deformation/multilateral_well

Poroelasticity (Multiphysics Coupling)

The **Poroelasticity** multiphysics coupling node (N) links bidirectionally the Solid Mechanics and Darcy's Law interfaces to account for poroelastic deformation.

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 porol.

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 poroelasticity coupling, or select All domains as needed.

When **Poroelasticity** is added as an effect of adding a Poroelasticity interface, the selection is the same as for the participating physics interfaces.

Only domains that are active in the physics interfaces selected in the Coupled Interfaces section can be selected.

POROELASTIC COUPLING PROPERTIES

In the **Reference pressure level** field, enter a reference pressure p_{ref} (SI unit: Pa) at which the pore pressure does not affect the porous matrix deformation. The default value is 1 atm.

For the Biot-Willis coefficient list, the default is to take its value From material. Choose **User defined** to enter a Biot–Willis coefficient α_B (dimensionless) in the text field.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Solid** mechanics and Flow in porous media lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (macOS and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the Model Wizard or Add Physics window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Poroelasticity node from a physics interface. If the physics interface is removed from the Model Builder, for

example Darcy's Law is deleted, then the Flow in porous media list defaults to None as there is nothing to couple to.



If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the Solid mechanics or Flow in porous media lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the COMSOL Multiphysics Reference Manual.

The Poroelasticity, Large Deformation Interface

The multiphysics interface Poroelasticity, Large Deformation couples the Darcy's Law interface and the Solid Mechanics interface. Although the theory for the two Poroelastic interfaces Poroelasticity, Solid and Poroelasticity, Large Deformation quite differs as shown in Theory for the Poroelasticity Interfaces, the interface settings and the multiphysics interfaces look quite similar. The only obvious difference is that for large deformations, an Elastic Predeformation node within the Solid Mechanics interface is active on all domains to track large deformations in the porous matrix. This feature forces the check box **Include geometric nonlinearity** in the solver settings to be checked.

For more information about the interface settings and the settings for the multiphysics node, see The Poroelasticity, Solid Interface and Poroelasticity (Multiphysics Coupling).





- Elastic Predeformation in the Structural Mechanics Module User's Guide
- Modeling Geometric Nonlinearity in the Structural Mechanics Module User's Guide



The Multiphysics interface **Poroelasticity**, **Large Deformation** is only available with some COMSOL products. For a detailed overview of the functionality available in each product, visit

https://www.comsol.com/products/specifications/

Theory for the Multiphase Flow in Porous Media Interface

The model equations that are solved in the **Multiphase Flow in Porous Media** interface are based on the mass conservation of each phase and on an extended Darcy's law. The mass conservation equation for each phase is given by

$$\frac{\partial}{\partial t} (\varepsilon_{\mathbf{p}} \rho_{i} s_{i}) + \nabla \cdot (\rho_{i} \mathbf{u}_{i}) = Q_{i}$$
 (8-14)

where ε_p (dimensionless) is the porosity, and the vector \mathbf{u}_i should be interpreted as the volumetric flux of phase i (SI unit m³/(m²·s) or m/s). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_{i} = -\frac{\kappa_{ri}}{\mu_{i}} \kappa(\nabla p_{i} - \rho_{i} \mathbf{g})$$
 (8-15)

where κ denotes the permeability (SI unit: m^2) of the porous medium, \mathbf{g} the gravitational acceleration vector (SI unit m/s^2), and μ_i the dynamic viscosity (SI unit: $kg/(m \cdot s)$), p_i the pressure field (SI unit: Pa), and κ_{ri} the relative permeability (dimensionless) of phase i, respectively. The phase pressures p_i are related through the capillary pressure functions $p_{c_{ii}}$:

$$p_i - p_j = p_{c_{ij}}(s_1, ..., s_N) \qquad i \neq j$$
 (8-16)

One phase pressure can be chosen independently so that N-1 capillary pressure relations are needed to define the other phase pressures. In addition it is assume that all phases together fill the pore space completely, so that we have

$$\sum_{i=1}^{N} s_i = 1 \tag{8-17}$$

Pressure-Saturation Formulation

The algebraic relations in Equation 8-16 and Equation 8-17 allow for a reduction of the number of dependent variables. An often used way is to eliminate N-1 phase pressures and one of the saturations. This results in a so-called pressure-saturation

formulation (Ref. 3). The procedure in the Multiphase Flow in Porous Media interface is to pick one of the phases, let us say phase i_c , then express the volume fraction, s_i , of this phase in terms of the volume fractions of the other phases and in addition to use the pressure, p_i , of this phase to define the other phase pressures:

$$s_{i_{c}} = 1 - \left(\sum_{i=1, i \neq i_{c}}^{N} s_{i}\right)$$
 (8-18)

$$p_i = p_{i_c} + p_{c_{ii}}(s_1, ..., s_N)$$
 for $i \neq i_c$ (8-19)

The equations for the volume fractions s_i , $(i \neq i_c)$ are given by Equation 8-14 and Equation 8-15. To arrive at an equation for p_i , the conservation equations of all phases are summed. This results in

$$\frac{\partial}{\partial t} \left(\varepsilon_{p} \sum_{i=1}^{N} \rho_{i} s_{i} \right) + \nabla \cdot \left(\sum_{i=1}^{N} \rho_{i} \mathbf{u}_{i} \right) = Q_{\text{tot}}$$
 (8-20)

where the total mass source Q_{tot} is given by

$$Q_{\text{tot}} = \sum_{i=1}^{N} Q_i \tag{8-21}$$

The equations for the volume fractions s_i are solved in the **Phase Transport in Porous** Media interface (see Equation 6-99 and Equation 6-100). The Equation 8-20 for the pressure field $p_{i_{k}}$, needed as an input to the Phase Transport in Porous Media interface, is solved for in the Darcy's Law interface: the Multiphase Flow in Porous Media multiphysics coupling interface replaces the equation

$$\frac{\partial}{\partial t} (\varepsilon_{\mathbf{p}} \rho_{i_c}) + \nabla \cdot (\rho_{i_c} \mathbf{u}_{\mathbf{d}}) = Q_{\mathbf{m}} \quad \text{where} \quad \mathbf{u}_{\mathbf{d}} = -\frac{1}{\mu_{i_c}} \kappa (\nabla p_{i_c} - \rho_{i_c} \mathbf{g})$$
(8-22)

which is originally implemented in the **Darcy's Law** interface, with Equation 8-20 by adding the following terms to the left-hand side of Equation 8-22:

$$\frac{\partial}{\partial t} \left(\varepsilon_{p} \sum_{i=1}^{N} \rho_{i} s_{i} - \varepsilon_{p} \rho_{\text{tot}} \right) + \nabla \cdot \left(\sum_{i=1}^{N} \rho_{i} \mathbf{u}_{i} - (\rho_{\text{tot}} \mathbf{u}_{d}) \right)$$
(8-23)

and by setting the right-hand side $Q_{
m m}$ to be equal to $Q_{
m tot}$.

Furthermore, the **Multiphase Flow in Porous Media** multiphysics coupling interface couples the user inputs for the porosity and permeability of the porous matrix in the **Darcy's Law** interface to the corresponding user input fields in the **Phase and Porous Media Transport Properties** feature, and couples the pressure field computed for in the **Darcy's Law** interface to the user input field for the pressure of the phase computed from the volume constraint.

Note that when the hydraulic conductivity of a domain is specified in the **Darcy's Law** interface (instead of the permeability), the coupled **Phase and Porous Media Transport Properties** feature is supplied with a permeability that is computed using a reference kinematic viscosity of $1.004*10^{-6}$ m²s⁻¹ (kinematic viscosity of water at 293.15 K).

In the other direction, the multiphysics coupling node provides the averaged density (denoted by ρ_{tot} in Equation 8-23 above) and effective viscosity to the **Darcy's Law** interface.

Mass Source

When adding a Mass Source node in the coupled Phase Transport interface, it is by default assumed that the net mass source of all phases, Q_{tot} , equals zero. This implies

$$Q_{i_c} = -\sum_{i=1, i \neq i_c}^{N} Q_i$$
 (8-24)

However, when mass is transferred from or to phases not accounted for in the phase transport interface — for instance, when mass is released or absorbed by the solid part of the porous matrix — select the **Mass transfer to other phases** check box. In this case the mass source for the phase calculated from the volume constraint should also be specified, and the net total mass source $Q_{\rm tot}$ is supplied as a right-hand side to the Darcy Equation 8-20 for p_i .

Boundary Conditions

When supplying boundary conditions for the coupled **Phase Transport in Porous Media** and **Darcy's Law** interfaces, bear in mind that the **Pressure** boundary condition in the **Darcy's Law** interface affects the pressure of the phase from the volume constraint, p_{i_c} . If the pressure of another phase needs to supplied, then take into account the capillary pressure.

Since the coupled Darcy's Law interface uses the conservation equation for the total mass (Equation 8-20) to solve for p_{i_a} , the Mass Flux boundary condition in the Darcy's **Law** interface should be used to prescribe the mass flux of all phases together.

If the mass flux of the phase computed from the volume constraint needs to be prescribed at a boundary, and the total mass flux is not known a priori, it might be necessary to compute for the total mass flux in the form of a Lagrange multiplier by using the weak constraint formulation for the pressure boundary condition in the Darcy's Law interface.

References

- 1. J. Bear, Dynamics of Fluids in Porous Media, Elsevier Scientific Publishing, 1972.
- 2. Z. Chen, G. Huan, and Y. Ma, Computational Methods for Multiphase Flows in Porous Media, Philadelphia: Society for Industrial and Applied Mathematics, 2006.
- 3. R. Helmig, Multiphase Flow and Transport Processes in the Subsurface A Contribution to the Modeling of Hydrosystems, Springer-Verlag, 1997.

The Multiphase Flow in Porous Media Interface

The Multiphase Flow in Porous Media interface () combines the Darcy's Law interface with the Phase Transport in Porous Media interface to model the flow and transport of multiple immiscible phases in a porous medium.

When a predefined Multiphase Flow in Porous Media interface is added from Porous Media and Subsurface Flow branch () of the Model Wizard or Add Physics window, **Phase Transport** and **Darcy's Law** interfaces are added to the Model Builder. In addition, the Multiphysics node is added, which automatically includes the Multiphase Flow in Porous Media multiphysics coupling.

On the Constituent Physics Interfaces

The Phase Transport in Porous Media interface is used to simulate the transport of immiscible multiple species in a porous medium and solves for their averaged volume fractions (also called saturations). The interfaces between the different phases are not tracked explicitly, although microscopic interfacial effects are taken into account in the macroscopic equations through the capillary pressure functions.

The Darcy's Law interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example Multiphase Flow in Porous Media, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Phase Transport** and **Darcy's Law** interfaces are added, an empty Multiphysics node appears in the model tree. You can choose from the available coupling features but the settings in the constituent interfaces are not modified.

The Multiphase Flow in Porous Media multiphysics coupling node () links bidirectionally the Phase Transport in Porous Media and Darcy's Law interfaces.

SETTINGS

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

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>. <variable name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is mfpm1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the Selection list to choose specific domains to define the multiphase flow coupling, or select All domains as needed.

When Multiphase Flow in Porous Media is added as an effect of adding a Multiphase Flow in Porous Media interface, the selection is the same as for the participating physics interfaces.

Only domains that are active in the participating physics interfaces (which are chosen from the **Coupled Interfaces** selection list) can be selected.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The Phase transport and Flow in porous media lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the Physics ribbon (Windows users), Physics contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the Model Wizard or Add Physics window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Multiphase Flow in Porous Media node from a physics interface. If the physics interface is removed from the **Model** Builder, for example Darcy's Law is deleted, then the Flow in porous media list defaults to **None** as there is nothing to couple to.

Please find related information under



- The Phase Transport Interfaces and
- Theory for the Phase Transport Interfaces

in the CFD Module User's Guide.

Well (Multiphysics Coupling)

The Multiphase Flow in Porous Media () interface contains an optional Well multiphysics coupling feature on points (in 2D) or edges (in 3D). The Well coupling node is intended to model injection or production wells and links bidirectionally the Phase Transport in Porous Media and Darcy's Law interfaces.

The Subsurface Flow Module license is required to use this coupling feature (see https://www.comsol.com/products/specifications/).

SETTINGS

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

The default **Name** (for the first **Well** multiphysics coupling feature in the model) is wellmpp1.

POINT OR EDGE SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific points or edges, or select **All points** or **All edges** as needed.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the Phase transport or Flow in porous media lists

WELL

Select whether the well is a production or injection well: for an injection well positive mass fluxes signify inflowing fluxes and for a production well positive mass fluxes are outflowing fluxes.

Either specify the total **Total mass flow rate** M_0 (SI unit: kg/s), the **Total mass flow rate** per unit length M_1 (SI unit: kg/(m·s)), the Pressure p_0 (SI unit: Pa), the Pressure head $H_{\rm p0}$ (SI unit: m), or the **Hydraulic head** H_0 (SI unit: m). The elevation D used to convert the hydraulic head to a pressure, is defined by the gravity effects in the coupled Darcy's Law interface.

Select the **Specify well diameter** check box to define the **Well diameter** $d_{\mathbf{w}}(\mathrm{SI~unit:m})$. This averages the mass source on the boundary of a cylinder around the line. This option avoids obtaining an increasing pressure value at the line when meshing finer than this diameter. It makes use of the circavg operator.

If the well diameter is defined, the option to specify the **Total mass flux** N_0 (SI unit: $kg/(m^2 \cdot s)$) is also available.

PHASES

The number of **Phase** sections depends on the number of phases defined in the coupled Phase Transport in Porous Media interface: the number of sections is equal to the number of phases not computed from the volume constraint, which is in turn equal to the number of phases defined in the coupled Phase Transport in Porous Media interface minus one.

Specify the boundary condition for each phase not computed from the volume constraint. You can choose to enter a value for the Mass flow rate $M_{0,i}$ (SI unit: kg/s), the Mass flow rate per unit length $M_{\mathrm{l},i}$ (SI unit: kg/(m·s)), or the Volume fraction $s_{\mathrm{0},i}$ (dimensionless). If the well diameter is specified, the option to specify the Mass flux $N_{0,i}$ (SI unit: $kg/(m^2 \cdot s)$) is also available. For a production well, you can additionally choose the Outflow option. For an injection well you can additionally choose to specify the Fraction of total volumetric flow rate $s_{0,i}$ (dimensionless).

Fraction of total volumetric flow rate

When the Fraction of total volumetric flow rate $s_{0,i}$ is specified for a phase, a mass flow rate per unit length $M_{l,i}$ is supplied for that phase, which is given by

$$M_{l,i} = \rho_i s_{0,i} V_l \tag{8-25}$$

where V_1 is the total volumetric flow rate per unit length, which is computed as follows: assume that there are N phases, and that phase 1 is the phase computed from the

volume constraint, that for phases i, for i = 2, ..., p, the fraction of total volumetric flow rate $s_{0,i}$ is supplied, and that for the phases i, for i = p+1, ..., N, the mass flow rate per unit length $M_{1,i}$ is given. Then V_1 can be computed from the relation

$$V_{1} = \frac{M_{1,1}}{\rho_{1}} + \sum_{i=2}^{p} V_{1} s_{i,0} + \sum_{i=p+1}^{N} \frac{M_{1,i}}{\rho_{i}}$$
 (8-26)

where the mass flow rate $M_{l,1}$ for the phase computed from the volume constraint is given by

$$M_{l, 1} = M_{l} - \sum_{i=2}^{p} V_{l} \rho_{i} s_{i, 0} - \sum_{i=p+1}^{N} M_{l, i}$$
 (8-27)

Note that the total mass flow rate per unit length M_1 is readily available when any of the Total mass flow rate, Total mass flow rate per unit length, or the Total mass flux options is chosen. Furthermore, the total mass flow rate per unit length M_1 is also available as a Lagrange multiplier in case any of the Pressure, the Pressure head, or the Hydraulic head is given, as these conditions are implemented as weak constraints. For the mass flow rates per unit length $M_{1,i}$ of the individual phases, it holds similarly that they are readily available when any of the Mass flow rate, Mass flow rate per unit length, or the Mass flux options are chosen, and that for the Volume fraction option, implemented as a weak constraint, the mass flow rate per unit length $M_{1,i}$ is computed as a Lagrange multiplier.

Outflow

When the **Outflow** option is specified for a phase s_i , an outflowing mass flow rate per unit length $M_{l,i}$ is supplied for that phase, which is given by

$$M_{l,i} = \frac{\rho_i \kappa_{ri}}{\lambda_r \mu_i} M_l$$
 with $\lambda_r = \sum_{i=1}^N \frac{\rho_i \kappa_{ri}}{\mu_i}$ (8-28)

where κ_{ri} denotes the relative permeability of phase i.

The Reacting Flow in Porous Media Interface

The Reacting Flow in Porous Media, Transport of Diluted Species interface (🔝) is used to study the flow and chemical composition of a gas or liquid moving through the interstices of a porous medium.

It combines the Brinkman Equations and Transport of Diluted Species in Porous Media interfaces. The Reacting Flow, Diluted Species multiphysics coupling feature, which is added automatically, couples the fluid flow and mass transport.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi, and 3D.

Detailed information is available in the section The Reacting Flow in Porous Media Multiphysics Interfaces of the Chemical Reaction Engineering User's Guide.

The Nonisothermal Flow, Brinkman Equations Interface

The Multiphysics coupling Nonisothermal Flow, Brinkman Equations is used to model heat transfer and flow in porous media where both the temperature and flow fields have to be coupled. Here, the nonlocal couplings between porous media flow and heat transfer are set up automatically.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

When the Brinkman Equations multiphysics interface is chosen from the Fluid Flow>Nonisothermal Flow branch of the Model Wizard or Add Physics windows, the Heat Transfer in Porous Media and the Brinkman Equations interfaces are added to the Model Builder. In addition, the Multiphysics node is added, which automatically includes the multiphysics coupling feature Nonisothermal Flow.

Furthermore, a Porous Material node with a Fluid and a Solid subnode is automatically generated under Component > Materials.

Settings for the Brinkman Equations Interface and the Coupling Feature

When physics interfaces are added using the predefined couplings, specific settings are included with the physics interfaces and the coupling features.

In this case, in the **Brinkman Equation** Settings, the **Compressibility** option is set to Weakly compressible flow. The Density ρ in the Porous Medium > Fluid subnode is automatically set to the variable from the **Nonisothermal Flow** multiphysics coupling feature.

For Heat Transfer in Porous Media in the Porous Medium > Fluid subnode, the Absolute pressure, $p_{\rm A}$ (Model Input section of the Porous Medium > Fluid node) and the Velocity field, u (Heat Convection section) are automatically set to the variables from the Nonisothermal Flow multiphysics coupling feature.

Note that if the physics interfaces are added one at a time, followed by the coupling feature, these modified settings may not be automatically included.

To get all the modified settings presented below automatically, you may right-click the component node, select Add Multiphysics, and add the Nonisothermal Flow coupling feature.

- The Brinkman Equations Interface
- The Heat Transfer in Porous Media Interface in the Heat Transfer Module User's Guide



- The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces in the CFD Module User's Guide
- Heat Transfer and Fluid Flow Coupling in the Heat Transfer Module User's Guide
- The Multiphysics Branch in the COMSOL Multiphysics Reference Manual.

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