

# Porous Media Flow Module

User's Guide



#### Porous Media Flow Module User's Guide

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### Introduction

The Porous Media Flow Module is an optional add-on package for COMSOL Multiphysics<sup>®</sup> designed to assist you to model transport processes in porous media.

This chapter introduces you to the capabilities of this module and includes a summary of the physics interfaces as well as information about where you can find additional documentation and model examples. The last section is a brief overview with links to each chapter in this guide.

- About the Porous Media Flow Module
- Overview of the User's Guide

### About the Porous Media Flow Module

#### In this section:

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

#### Why Porous Media Flow Is Important for Modeling

Porous media are encountered in many natural as well as manufactured systems. The need for advanced porous media modeling spans many industries and application areas like processes in fuel cells, paper-pulp drying, food production and safety, filtration, concrete, ceramics, moisture absorbents, textiles, paint drying, polymer composites, and detergent tablets. The most well-known natural porous media involving multiphase flow and transport are soils, aquifers, and oil and gas reservoirs. However, such processes also occur in biological tissues and plants. Recently, there has been growing interest in the biomechanics of porous tissues, engineered tissues, and in-tissue drug delivery.

Many of these porous systems are extremely complex. Therefore, the traditional concepts, models, and algorithms developed for porous media in the geosciences are not directly applicable and there is a very strong need for tailored models. Multiphysics couplings are essential to capture the effects of porous media on transport processes.

#### How the Porous Media Flow Module Helps Improve Your Modeling

The Porous Media Flow Module is an optional package that extends the COMSOL Multiphysics modeling environment with customized physics interfaces and functionality optimized for the analysis of transport processes in porous media. It combines physics interfaces for fundamental processes and links to COMSOL Multiphysics and the other modules for structural mechanics and electromagnetics analyses. Important in industrial porous media flow, the heat transfer and chemical

transport interfaces explicitly account for physics in the liquid, solid, and gas phases and include the possibility to model thermal nonequilibrium. The physics interfaces for heat transfer 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 along thin layers and fractures.

This 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 accounts for chemical transfer in solid, liquid, and gas phases for free and porous media flows. The Porous Media Flow Module Application Library includes a number of examples linking these physics interfaces together.

Predefined multiphysics couplings make it possible to conveniently model poroelastic effects and multiphase transport processes.

#### The Porous Media Flow Module Physics Interface Guide

The Porous Media Flow Module extends the functionality of the physics interfaces of the base package of COMSOL Multiphysics with respect to the different physical aspects that are important for modeling porous media, like heat transfer in porous media and layered materials, diffusion and reactions of chemical species in porous media, and fluid flow in porous media. It also contains predefined multiphysics couplings, for example, with structural mechanics to simulate poroelasticity or with free flow interfaces. The table below lists all the interfaces specifically available with this module.

In the COMSOL Multiphysics Reference Manual:

2

· 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 Tr	anspoi	rt	DII IENOION	
	,		ı	ı
Transport of Diluted Species <sup>I</sup>	:=*	tds	all dimensions	stationary; time dependent
Transport of Diluted Species in Porous Media	S	tds	all dimensions	stationary; time dependent
Transport of Diluted Species in Fractures	<b>E</b>	dsf	3D, 2D, 2D axisymmetric	stationary; time dependent
Moisture Transpo	rt			
Moisture Transport in Air	<b>%</b>	mt	all dimensions	stationary; time dependent
Moisture Transport in Porous Media	<b>***</b>	mt	all dimensions	stationary; time dependent
Moisture Transport in Building Materials	<b>***</b>	mt	all dimensions	stationary; time dependent
Moisture Transport in Solids	<b>.</b> ₩	mts	all dimensions	stationary; time dependent
Moisture Flow				
Laminar Flow	<b>*</b>	_	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way Moisture Flow; time dependent, one-way Moisture Flow
Porous Media Flow		_	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way Moisture Flow; time dependent, one-way Moisture Flow
Reacting Flow				
Laminar Flow, Diluted Species	<b>*</b>		3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE							
Reacting Flow in	Porous	Media									
Transport of Diluted Species		_	3D, 2D, 2D axisymmetric	stationary; time dependent							
Fluid Flow	Fluid Flow										
Single-Phase Flow	1										
Creeping Flow	==	spf	3D, 2D, 2D axisymmetric	stationary; time dependent							
Laminar Flow	<b>*</b>	spf	3D, 2D, 2D axisymmetric	stationary; time dependent							
Multiphase Flow											
Two-Phase Flow, Le	vel Set										
Two-Phase Flow, Level Set, Brinkman Equations		_	3D, 2D, 2D axisymmetric	time dependent with initialization							
Phase Transport		'	'	'							
Phase Transport	<b>*</b>	phtr	all dimensions	stationary; time dependent							
Phase Transport in Porous Media		phtr	all dimensions	stationary; time dependent							
Phase Transport in Free and Porous Media Flow		phtr	all dimensions	stationary; time dependent							
Porous Media and	l Subsu	ırface Flo	w								
Brinkman Equations	Ō	br	3D, 2D, 2D axisymmetric	stationary; time dependent							
Darcy's Law	<b>⊗</b>	dl	all dimensions	stationary; time dependent							

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Layered Darcy's Law		ldl	3D	stationary; time dependent
Fracture Flow	R	ff	3D, 2D, 2D axisymmetric	stationary; time dependent
Richards' Equation	<b>**</b>	dl	all dimensions	stationary; time dependent
Multiphase Flow in Porous Media	S.	_	all dimensions	stationary; time dependent
Free and Porous Media Flow, Brinkman		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Darcy		_	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Fl	ow	·		
Brinkman Equations	<b>(</b>	_	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF
Heat Transfer		·		
Heat Transfer in Solids	<b>/</b>	ht	all dimensions	stationary; time dependent
Heat Transfer in Fluids <sup>I</sup>	<b>∫</b> ≋	ht	all dimensions	stationary; time dependent
Heat Transfer in Solids and Fluids <sup>I</sup>	<b>∫</b> ≅	ht	all dimensions	stationary; time dependent
Thin Structures	•			
Heat Transfer in Fractures	<b>)</b> 🚱	htlsh	3D, 2D, 2D axisymmetric	stationary; time dependent; thermal perturbation, frequency domain
Heat and Moisture Transport				

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE	
Moist Air	<b>/≋</b>		all dimensions	stationary; time dependent; thermal perturbation, frequency domain	
Moist Porous Media	<b>(83</b> )	_	all dimensions	stationary; time dependent; thermal perturbation, frequency domain	
Building Materials	<b>(8</b> )		all dimensions	stationary; time dependent; thermal perturbation, frequency domain	
Heat and Moisture Flow					
Laminar Flow	<b>\rightarrow</b>	_	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way Moisture Flow; time dependent, one-way Moisture Flow	
Porous Media Flow	<b>(S</b> )	_	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way Moisture Flow; time dependent, one-way Moisture Flow	
Porous Media					
Heat Transfer in Porous Media	<b>(S</b> )	ht	all dimensions	stationary; time dependent	
Local Thermal Nonequilibrium	<b>/S</b>	ht	all dimensions	stationary; time dependent; thermal perturbation, frequency domain	
Heat Transfer in Packed Beds	<b>  S</b>	ht	all dimensions	stationary; time dependent; thermal perturbation, frequency domain	
Structural Mechanics					
Poroelasticity					
Poroelasticity, Solid <sup>2</sup>	<b>♦</b>		3D, 2D, 2D axisymmetric	stationary; time dependent	

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Poroelasticity, Large Deformation, Solid <sup>2,3</sup>	<b>\$</b>	_	3D, 2D, 2D axisymmetric	stationary; time dependent
Poroelasticity, Layered Shell <sup>2,4</sup>		_	3D	stationary; time dependent
Unsaturated Poroelasticity <sup>2,3</sup>	<b>*</b>	_	3D, 2D, 2D axisymmetric	stationary; time dependent
∆∪ Mathematics				
Level Set	<b>\$\$</b> \$\$\$	ls	all dimensions	time dependent with phase initialization
Level Set in Porous Media	<b>S</b>	ls	all dimensions	time dependent with phase initialization

This physics interface is included with the core COMSOL Multiphysics software 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.

<sup>&</sup>lt;sup>2</sup> This physics interface is a predefined multiphysics coupling that automatically adds all the physics interfaces and coupling features required.

<sup>&</sup>lt;sup>3</sup> Requires the addition of the Structural Mechanics Module.

<sup>&</sup>lt;sup>4</sup> Requires the addition of the Composite Materials Module and the Structural Mechanics Module.

#### The Porous Media Flow Module Study Availability

All the physics interfaces included with the module have the Stationary and Time Dependent preset studies available. The Heat Transfer in Fractures Interface additionally includes the Thermal Perturbation, Eigenfrequency study to compute eigenmodes and eigenfrequencies of linearized models around an equilibrium steady-state temperature field. 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 Material 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 ( 2 ). This is called *topic-based* (or *context*) *belp*.

To open the **Help** window:

 In the Model Builder, Application Builder, or Physics Builder, click a node or window and then press F1.

Win

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

Opening the Documentation Window

To open the **Documentation** window:

Win

- · Press Ctrl+F1.
- From the File 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 ( iii):



From the File menu, select Application Libraries.

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



From the File or Windows menu, select Application Libraries.



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

#### CONTACTING COMSOL BY EMAIL

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

#### COMSOL ACCESS AND TECHNICAL SUPPORT

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

#### COMSOL ONLINE RESOURCES

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

### Overview of the User's Guide

The Porous Media 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 Multiphysics 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 AND THE MULTIPHASE FLOW BRANCH

The Single- and Multiphase Flow Interfaces section describes the Laminar and Creeping Flow interfaces. The Phase Transport Interfaces are used to model the transport of multiple immiscible phases in free and porous media flow. They are described in the CFD Module User's Guide and just referenced here.

#### THE POROUS MEDIA FLOW BRANCH

The 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 intended for flow in porous media that is relatively
- The Richards' Equation Interface is intended for variably saturated systems.
- The Fracture Flow Interface is a special application of Darcy's law for modeling flow in fractures.
- The Layered Darcy's Law Interface is intended for flow in porous media that is relatively slow.

- The Brinkman Equations Interface is intended for fast flow in porous media flow.
- The Free and Porous Media Flow, Brinkman Interface and The Free and Porous Media Flow, Darcy Interface are intended for modeling fluid flow in systems with both free and porous media flow.

#### THE CHEMICAL SPECIES TRANSPORT BRANCH

The 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.

are two different interfaces that can be used to model moisture transport in building materials and moisture transport in air, respectively, taking into account the different transport mechanisms.

#### THE HEAT TRANSFER BRANCH

The 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

The Local Thermal Nonequilibrium Interface solves two heat transfer equations in the solid and fluid phases, to model heat transfer in porous media for which the solid and fluid temperatures are not in equilibrium.



When your license includes the Porous Media Flow Module plus the Chemical Reaction Engineering Module or Heat Transfer Module, 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 section 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 Moisture Flow Interface couples moisture transport in air by vapor diffusion and convection with a laminar flow interface.

The Heat and Moisture Transport Interfaces couple heat transfer and moisture transport in building materials or in moist air, respectively.

The Heat and Moisture Flow Interface combines the functionalities of three different interfaces: Laminar flow, Moisture Transport in Air, and Heat Transfer in Moist Air.

The Reacting Flow in Porous Media Interface combines the Brinkman equations with the Transport of Diluted Species interface.

## Porous Media Flow Modeling

This chapter introduces you to the modeling of flows in porous media.

#### In this chapter:

- What Is a Porous Medium?
- About Darcian and Non-Darcian Flow
- Permeability Models
- Mass and Momentum Conservation in Porous Media
- Ambient Properties

### What Is a Porous Medium?

A porous material consists of a solid structure (porous matrix) with voids (pores) filled with a liquid or gas. Porous materials are found in all sizes and across a wide range of applications - from nanomaterials to porous reactors, for cooling of electronic components to large scale geotechnical applications. What they all have in common is that the total size of the material is much bigger than the mean pore diameter, so that a macroscopic approach must be used to model the applications.

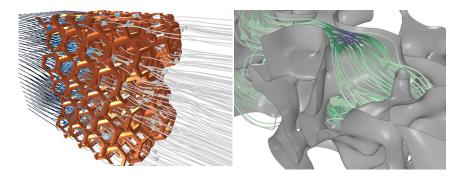


Figure 2-1: Flow through porous structures.

If it is possible to calculate averaged values from the simulation on a microscopic scale (Figure 2-1), which are also representative for any other section, the modeled section is called a representative volume element (RVE). Two variables mainly characterize the porous material: The porosity describes the ratio of void/pore volume to total volume

$$\varepsilon_{\rm p} = \frac{V_{\rm V}}{V_{\rm tot}}$$

and the permeability  $\kappa$  (m<sup>2</sup>) specifies the ability of a fluid to pass through it.

### About Darcian and Non-Darcian Flow

The basic law that describes the flow in porous materials is Darcy's law. It describes a linear relationship between the velocity field  $\mathbf{u}(m/s)$  and the gradient of the pressure p(Pa).

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{2-1}$$

This is only valid for very low velocities or at low Reynolds numbers (Re < 10)

2

See the section The Reynolds Number in the COMSOL Multiphysics Reference Manual.

In case of relatively fast flow (Re > 10) or relatively high Knudsen numbers (Kn > 0.1) Darcy's linear relation between velocity and pressure drop is no longer valid. Therefore, different Permeability Models have been introduced to capture these effects. A general form of the nonlinear relationship of pressure gradient to velocity can be written as

$$-\nabla p = \frac{\mu}{\kappa} \mathbf{u} + \beta \rho \mathbf{u} |\mathbf{u}| \tag{2-2}$$

The flow regime through a packed bed may be identified from the Reynolds number of the bed. According to textbooks, for Reynolds numbers Re < 10 the flow can be described by Kozeny-Carman equation (Darcian flow). For 10 < Re < 1000, which is sometimes called the transitional regime, the flow is better described by the non-Darcian Ergun equation, and for Re > 1000 Ergun's equation can be approximated by the Burke-Plummer equation for turbulent flows.

### Permeability Models

Different models can define the capacity of the porous medium to transmit flow. Some use the permeability,  $\kappa$  (SI unit: m<sup>2</sup>), and the viscosity of the fluid,  $\mu$  (SI unit: Pa·s); others use the hydraulic conductivity, K (SI unit: m/s). Several relationships have been established to describe Darcian and non-Darcian flow through different porous materials.

#### PERMEABILITY

The capacity of the porous medium to transmit flow cannot be described by porosity alone, as the shape and orientation of the pores is also an important factor. This is described by the permeability  $\kappa$ . For an isotropic medium  $\kappa$  is a scalar quantity. Often porous materials are anisotropic and  $\kappa$  then is a tensor.

There is also the term relative permeability, which is relevant for multiphase flow in porous media applications.

2

For modeling multiphase flow in porous media The Multiphase Flow in Porous Media Interface is available. For flow through unsaturated porous media, also The Richards' Equation Interface is available.

#### HYDRAULIC CONDUCTIVITY

The hydraulic conductivity represents both fluid and solid properties. If the model is defined using the hydraulic conductivity as in:

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

Equation 2-1 changes to

$$\mathbf{u} = -\frac{\mathbf{K}}{\rho g} \nabla p \tag{2-3}$$

#### KOZENY-CARMAN

The Kozeny-Carman equation describes the flow through granular soils and packed beds by estimating the permeability of the porous medium from the porosity  $\epsilon_{\rm p}$  and average particle diameter  $d_p$  (see, for example, Ref. 5).

$$\kappa = \frac{d_{\rm p}^2}{180} \frac{\varepsilon_{\rm p}^3}{(1 - \varepsilon_{\rm p})^2}$$

#### ERGUN

The Ergun equation is an extension of Kozeny-Carman equation to higher Reynolds numbers (Re > 10), where Darcy's linear relation between pressure drop and velocity is no longer valid. In Ergun equation the linear relation between pressure drop and velocity is augmented by a quadratic term. The pressure drop (Ref. 6) in Ergun's equation is given by:

$$-\nabla p = \frac{150}{d_{\rm p}^2} \frac{(1 - \varepsilon_{\rm p})^2}{\varepsilon_{\rm p}^3} \mu \mathbf{u} + \frac{1.75}{d_{\rm p}} \frac{(1 - \varepsilon_{\rm p})}{\varepsilon_{\rm p}^3} \rho \mathbf{u} |\mathbf{u}|$$

Here,  $d_{\mathrm{p}}$  is the effective (average) particle diameter in the porous medium and  $\varepsilon_{\mathrm{p}}$  is the porosity. With definitions of permeability  $\kappa$  and parameter  $\beta$  (SI unit 1/m) as

$$\kappa = \frac{d_p^2}{150} \frac{\varepsilon_p^3}{(1 - \varepsilon_p)^2} \tag{2-4}$$

and

$$\beta = \frac{1.75}{d_{\rm p}} \frac{(1 - \varepsilon_{\rm p})}{\varepsilon_{\rm p}^3} \tag{2-5}$$

we get Equation 2-2 and Ergun's velocity can then be calculated as

$$\mathbf{u} = -\frac{\kappa}{\mu} \frac{2}{1 + \sqrt{1 + 4\left(\frac{\kappa}{\mu}\right)^2 \beta \rho |\nabla p|}} \nabla p$$

Using the Reynolds number Re and the friction factor  $f_p$  for packed beds

$$Re = \frac{d_{p}\rho|\mathbf{u}|}{(1-\varepsilon_{p})\mu}$$

$$f_{\rm p} = |\nabla p| \frac{d_{\rm p}}{\rho \mathbf{u}^2} \frac{\varepsilon_{\rm p}^3}{(1 - \varepsilon_{\rm p})} = \frac{150}{\text{Re}} + 1.75 ,$$

Ergun's velocity can alternatively be written as

$$\mathbf{u} = -\frac{\kappa}{\mu} \left( 1 - \frac{1.75}{f_{\rm p}} \right) \nabla p$$

From this expression, we observe that for low Reynolds numbers Re < 1 (or equivalently, high friction factors) the flow can be described by the linear Darcy's Law (Equation 2-1).

#### FORCHHEIMER

For increasing filter velocities (Re > 10), inertial effects and turbulent friction forces become significant. In the Forchheimer drag this is considered by adding an additional term to Darcy's law:

$$-\nabla p = \frac{\mu}{\kappa} \mathbf{u} + \frac{c_F}{\sqrt{\kappa}} \rho \mathbf{u} |\mathbf{u}|$$
 (2-6)

Here, the Forchheimer parameter  $c_F$  is dimensionless. The permeability  $\kappa$  is specified by the user and is not computed from porosity nor particle diameter as for Ergun's equation. If the parameter  $\beta$  is defined as

$$\beta = \frac{c_F}{\sqrt{\kappa}}$$

Equation 2-6 becomes equivalent to Equation 2-1.

#### BURKE-PLUMMER

The Burke-Plummer equation is applicable in flow regimes with Reynolds number Re > 1000. Here, the pressure drop is proportional to the square of the velocity:

$$\frac{\Delta p}{L} = \frac{1.75}{d_{\rm p}} \frac{(1 - \varepsilon_p)}{\varepsilon_p^3} \rho v^2$$

here, L is the length of the packed bed,  $\Delta p$  is the pressure drop  $d_{
m p}$  is the effective (average) particle diameter in the porous medium,  $\varepsilon_p$  is the porosity, and v is the velocity magnitude.

Using the same definition for the parameter  $\beta$  (SI unit 1/m) as in Ergun's equation (Equation 2-5) the pressure drop is related to the velocity as

$$\frac{\Delta p}{L} = \beta \rho v^2$$

which means that the velocity magnitude can be written in terms of the pressure gradient as

$$v = \sqrt{\frac{|\nabla p|}{\beta \rho}}$$

As flow travels from areas of higher pressure to areas of lower pressure, Equation 2-2 can be more generally written as

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

replacing

$$|\mathbf{u}| = v = \sqrt{|\nabla p|/\beta \rho}$$

we get an expression for the velocity field in terms of the pressure gradient

$$\mathbf{u} = -\frac{1}{\sqrt{\beta \rho |\nabla p|}} \nabla p$$

Note that the viscosity is not used to define the velocity as in Darcy's law, but only the fluid density, the porosity and particle diameter. Note also that the analytical friction factor for Burke-Plummer equation is  $f_p = 1.75$ . A small parameter is added inside the square-root to avoid division by zero when the pressure gradient approaches zero.

#### KLINKENBERG

The Klinkenberg effect becomes important for gas flows in porous media where the mean free path of the gas molecules is comparable to the pore dimensions. In this case, molecular collisions with the pore walls occur more often than collisions between molecules. To take this effect into account, Klinkenberg (Ref. 7) derived the following expression for the permeability:

$$\kappa = \kappa_{\infty} \left( 1 + \frac{b_K}{p_A} \right) \tag{2-7}$$

here,  $\kappa_{\infty}$  is the permeability of the gas at high pressure and density (Knudsen number 0.001 < Kn < 0.1),  $b_K$  is the Klinkenberg parameter (also called Klinkenberg slip factor, or gas slippage factor), whose default value is set to 1 kPa according to Ref. 8, and  $p_A$  is the absolute pressure as defined in the Darcy's Law interface  $(p_A = p + p_{ref})$ .

# Mass and Momentum Conservation in Porous Media

In this chapter:

- Mass Conservation
- Momentum Conservation

#### Mass Conservation

In a volume of pure fluid with density  $\rho$  and viscosity  $\mu$  the mass conservation is defined by the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{2-8}$$

with the fluid velocity  $\mathbf{v}$ . For an incompressible fluid it simplifies to:

$$\rho \nabla \cdot \mathbf{v} = 0$$

For a porous medium Equation 2-8 must be corrected by the porosity  $\varepsilon_p$  because the fluid volume is only a fraction of the total volume, hence

$$\frac{\partial \varepsilon_{p} \rho}{\partial t} + \nabla \cdot (\varepsilon_{p} \rho \mathbf{v}) = 0 \tag{2-9}$$

Note that  $\mathbf{v}$  refers to the velocity of the fluid within the pores also called seepage or interstitial velocity. More commonly used to describe the flow through a porous medium is the superficial velocity or Darcy velocity u:

$$u = \frac{Q}{A} \tag{2-10}$$

Q (SI unit: m/s) is the volume flow rate of the fluid and A(SI unit: m<sup>2</sup>) is the cross sectional area of the porous medium. The cross-sectional area for the pore spaces which is available for the fluid to flow is related to the porosity by  $A_{\epsilon} = \epsilon_p A$  such that the Darcy velocity and seepage velocity relate as follows:

$$\mathbf{u} = \varepsilon_{p} \mathbf{v} \tag{2-11}$$

And Equation 2-9 can be written as:

$$\frac{\partial \varepsilon_{p} \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

or when a volumetric mass source  $Q_{\rm m}({\rm SI~unit:~kg/m3/s})$  is present:

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

Note that  $Q_{\mathrm{m}}$  is a mass source per unit volume of the porous medium (not per unit pore volume).

### Momentum Conservation

There are numerous ways for deriving the momentum equation in porous media. Here, start from the assumption that the pressure drop in a fluid results from viscous losses only and transient and inertial effects are neglected:

$$\nabla p = \mathbf{f}_{\text{viscous}}$$

The pressure p is the fluid pore pressure and for low velocities the viscous force depends linearly on the velocity (Equation 2-10) according to  $\nabla p \sim \mathbf{u}$ . This relation is well known as Darcy's law (Equation 2-1). The situation becomes more complicated when transient and inertial effects must be considered. For a pure fluid the governing equations are the Navier Stokes equations (see the section General Single-Phase Flow Theory in the COMSOL Multiphysics Reference Manual). The momentum conservation (Equation 13-2) rewritten for the fluid in a porous medium reads:

$$\varepsilon_{p} \rho \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = \varepsilon_{p} (\nabla \cdot [-p\mathbf{I} + K]) + \varepsilon_{p} \mathbf{f}_{\text{viscous}}$$
 (2-12)

Remember that  $\mathbf{v}$  denotes the interstitial velocity and K is the stress tensor. Equation 2-12 describes the momentum conservation per unit volume of the porous medium. It is more common to formulate the equation in terms of Darcy velocity. Dividing by  $\varepsilon_p$  and using Equation 2-11 yields:

$$\frac{\rho}{\varepsilon_{p}} \left( \frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\varepsilon_{p}} (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot [-p\mathbf{I} + K] + \mathbf{f}_{\text{viscous}}$$

The pressure drop due to viscous losses is described in Equation 2-2 and one obtains

$$\frac{\rho}{\varepsilon_{p}} \left( \frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\varepsilon_{p}} (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot [-p\mathbf{I} + K] + (\mu \kappa^{-1} + \beta \rho |\mathbf{u}|) \mathbf{u}$$
 (2-13)

A mass source or sink term adds a momentum source/sink as well and adds the term  ${\mbox{-}\epsilon_p} Qv$  to the right hand side of Equation 2-12. In terms of Darcy velocity Equation 2-13 can be rewritten as

$$\frac{\rho}{\varepsilon_p} \left( \frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\varepsilon_p} (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot [-p\mathbf{I} + K] + \left( \mu \kappa^{-1} + \beta \rho |\mathbf{u}| - \frac{Q}{\varepsilon_p} \right) \mathbf{u}$$

with

$$Q = \frac{Q_{\rm m}}{\varepsilon_{\rm p}}$$

Thus it results in the Brinkman equations (Equation 4-35) used by the The Brinkman Equations Interface.

# Ambient Properties

The ambient data available under the **Definitions** branch come from the processing of measured data from ASHRAE Weather Data Viewer 5.0 (©2013 ASHRAE, www.ashrae.org. Used with permission.), ASHRAE Weather Data Viewer 6.0 (©2017 ASHRAE, www.ashrae.org. Used with permission.), and Weather Data Viewer 2021 (©2021 ASHRAE, www.ashrae.org. Used with permission.) given as frequencies of observations, monthly and hourly averaged for several past years of observation. They provide time-dependent weather conditions for about 8500 stations worldwide in terms of the dry bulb temperature, the dew-point temperature, the relative humidity, the wind speed, the absolute pressure, the precipitation rate, and the solar direct and diffuse irradiance.

#### In this section:

- Settings for the Ambient Properties
- · Processing of ASHRAE Data
- Ambient Data Interpolation
- · Ambient Variables and Conditions
- Use of Ambient Data From the Features



When no special mention is added, the term temperature stands for the dry bulb temperature. See Theory for Heat Transfer in Moist Air in the Heat Transfer Module User's Guide for the definition of the dry bulb temperature, dew-point temperature, and relative humidity.

# Settings for the Ambient Properties

To add an Ambient Properties node to any Component, in the Physics toolbar click Ambient Properties or right-click the Definitions node under the Component and choose Ambient Properties.

In the **Ambient Properties** node ( \*), you can define ambient variables to be available as inputs from several features: the temperature  $T_{amb}$ , the absolute pressure  $p_{amb}$ , the relative humidity  $\phi_{amb}$ , the wind velocity  $v_{amb}$ , and the direct and diffuse solar irradiances  $I_{sn,amb}$  and  $I_{sh,amb}$ .

2

See The Moisture Transport Features in the Heat Transfer Module User's Guide.

Three options are available for the definition of the **Ambient data**:

- When User defined (the default) is selected, the Temperature  $T_{\rm amb}$ , the Absolute pressure  $p_{\rm amb}$ , the Relative humidity  $\phi_{\rm amb}$ , the Wind velocity  $v_{\rm amb}$ , the Precipitation rate  $P_{0,{\rm amb}}$ , the Clear sky noon beam normal irradiance  $I_{\rm sn,amb}$ , and the Clear sky noon diffuse horizontal irradiance  $I_{\rm sh,amb}$  should be specified directly.
- When either Meteorological data (ASHRAE 2013) or Meteorological data (ASHRAE 2017) or Meteorological data (ASHRAE 2021) is selected, the ambient variables are computed from monthly and hourly averaged measurements, made over several years at weather stations worldwide. See Processing of ASHRAE Data for more information. Further settings for the choice of the location, time, and ambient conditions are needed; and additional input fields are displayed underneath.

#### Location

In this section you can set the location by choosing among more than 8000 weather stations worldwide. Three options are available for the selection of the **Weather station**:

- When From list is selected, click on the Set Weather Station button to open the
  Weather Station browser that allows you to select a Region, a Country, and a Station.
  The station details (World Meteorological Organization reference, location, and
  geographical coordinates) are displayed underneath.
- It is also possible to select a station **From reference** by entering the corresponding **World Meteorological Organization reference**, which is a 6-digit number.
- When Around location is selected, enter the Latitude and Longitude around which you
  want to find a station. Click on the Set Weather Station button to open the Weather
  Station browser with the first 100 nearest stations, sorted by increasing distance
  from the specified location. The distance is calculated in kilometers using the
  haversine formula without consideration for the elevation. When the selection is

performed, the station details (World Meteorological Organization reference, location, and geographical coordinates) are displayed underneath.

Q	A single country may be available for more than one region selection if it has stations spread over different regions. For example, United States of America is available in the <b>Country</b> list when either North America, Eurasia, or Oceania is selected in the <b>Region</b> list.
Q	When a station is selected <b>From list</b> or <b>Around location</b> , its World Meteorological Organization (WMO) reference is displayed in the user interface. The WMO references can also be retrieved from maps offered by third parties like the one available as of this product release on <a href="http://ashrae-meteo.info/">http://ashrae-meteo.info/</a> .
Q	When a station is selected <b>Around location</b> , the <b>Latitude</b> and <b>Longitude</b> are decimal values, positive in the northern hemisphere and at the east of the Prime Meridian respectively. Both must be given without a unit to avoid double conversion. This is because the latitude and longitude values are expected to represent degrees but the model's unit for angles may be different (for example, the SI unit for the angle is radians).

#### Time

The **Date** and **Local time** should be set by entering values or expressions in the **Day**, Month, Hour, Minute, and Second fields of the two tables.

If On is selected in the Specify year list, a value or expression for the Year should also be set. As the data are given as averages over several past years, this input is only used for the detection of leap years, in order to interpolate the data over the months.

For temporal studies, these inputs define the start time of the simulation. By default, the **Update time from solver** check box is selected, and the time is then automatically updated with the time from the solver to evaluate the variables by interpolation of the measured data. Clear this check box to manually set the time update.

2

See Ambient Data Interpolation for more information about the interpolation of data over months and hours.

See Processing of ASHRAE Data for more information about the data.

2

A time unit suitable for simulations over a day or a year may be set in the **Study Settings** section of the **Time Dependent** node, by using for example **h** for hour, **d** for day, or **a** for a year. See Using Units in the COMSOL Multiphysics Reference Manual for more details.

#### Ambient Conditions

Based on the measured data, several conditions are available for the **Temperature**, the Dew-point temperature, the Wind speed, and the Precipitation rate. The formula for each condition is recalled in Table 2-1, Table 2-2, and Table 2-3. The Average conditions correspond to weighted means of the measured data, whereas the other conditions are obtained by applying standard or modified deviations (Low, High, and User defined coefficient for deviation conditions), user defined corrections, or wind correlations to the average conditions; or by taking the minimum or maximum of the measured data (Lowest and Highest conditions). More information about these definitions can be found in Ambient Variables and Conditions.

TABLE 2-I: TEMPERATURE CONDITIONS.

$_{ m amb} = \langle T_{ m station} \rangle$
$_{ m amb} = \langle T_{ m station}  angle - \sigma_{T, m station}$
$_{ m amb}$ = $\langle T_{ m station}  angle$ + $\sigma_{T, m station}$
$_{\rm amb} = \min(T_{\rm station})$
$_{\rm amb} = \max(T_{\rm station})$
$c_{amb} = \langle T_{station} \rangle + c_{\sigma} \cdot \sigma_{T,station}$
$_{ m amb} = \langle T_{ m station} \rangle + \Delta T$
$_{ m amb} = \langle T_{ m station} \rangle + \Delta T_{ m wind}$
$r_{\rm amb} = \langle T_{\rm station} \rangle - \Delta T_{\rm wind}$

(I) These correlations are not related to the wind speed conditions described in Table 2-3.

TABLE 2-2: DEW-POINT TEMPERATURE CONDITIONS.

CONDITION	DEFINITION
Average	$DPT_{amb} = \langle DPT_{station} \rangle$
Low	$DPT_{amb} = \langle DPT_{station} \rangle - \sigma_{DPT,station}$
High	$DPT_{amb} = \langle DPT_{station} \rangle + \sigma_{DPT,station}$

TABLE 2-2: DEW-POINT TEMPERATURE CONDITIONS.

CONDITIO	N	DEFINITION
Lowest		$DPT_{amb} = min(DPT_{station})$
Highest		$DPT_{amb} = max(DPT_{station})$
TABLE 2-3:	WIND SPEED CONDITIONS.	
CONDITION		DEFINITION
Average		$v_{ m amb} = \langle v_{ m station} \rangle$
Low		$v_{ m amb} = \langle v_{ m station} \rangle - \sigma_{v,  m station}$
High		$v_{ m amb} = \langle v_{ m station} \rangle + \sigma_{v,  m station}$
Lowest		$v_{\rm amb} = \min(v_{\rm station})$
Highest		$v_{ m amb} = \max(v_{ m station})$
TABLE 2-4:	PRESSURE CONDITIONS.	
CONDITION		DEFINITION
Average		$P_{0,\mathrm{amb}} = \langle P_{0,\mathrm{station}} \rangle -$
Low		$P_{0,\text{amb}} = \langle P_{0,\text{station}} \rangle - \sigma_{P_{0,\text{station}}}$
High		$P_{0,\text{amb}} = \langle P_{0,\text{station}} \rangle + \sigma_{P_{0,\text{station}}}$
Lowest		$P_{0,\mathrm{amb}} = \min(P_{0,\mathrm{station}})$
Highest		$P_{0,\text{amb}} = \max(P_{0,\text{station}})$
<b>Q</b>	The conditions set for <b>Temperature</b> and <b>Dew-point temperature</b> should be consistent in order to keep the temperature larger than the dew-point temperature. However, all settings combinations are available, and the relative humidity is majored by 1 when necessary.	
	T	
	The sum of the Clear sky	noon beam normal irradiance and the Clear sky

# Processing of ASHRAE Data

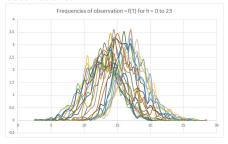
2

From frequencies of measured values, a weighted mean of the data and a standard deviation from the weighted mean are computed for each month. For the temperature,

variable ht.Is\_amb, defined as the Ambient solar irradiance.

noon diffuse horizontal irradiance is available through the postprocessing

more data are available and the weighted mean and standard deviation are also computed at each hour. Figure 2-2 shows an example of weighted mean computation for the diurnal temperature fluctuations from the initial data given as frequencies of observations.



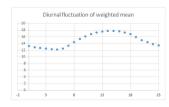


Figure 2-2: Computation of weighted mean from frequencies of observations for the diurnal fluctuations of temperature.

These values are used for the definition of different conditions, as detailed in Ambient Variables and Conditions.

All the monthly averaged observations except the solar irradiance are supposed to be made at the middle of each month. This time depends on the number of days in the month:

- Months with 31 days (January, March, May, July, August, October, December): data at the 16<sup>th</sup> at noon
- Months with 30 days (April, June, September, November): data at the 16<sup>th</sup> at midnight
- Months with 29 days (February, leap years): data at the 15<sup>th</sup> at noon
- Months with 28 days (February, other years): data at the  $15^{\mbox{th}}$  at midnight

In addition, the temperature observations are supposed to be made at the beginning of each hour (00:00 a.m. to 11:00 p.m.).

Finally, the solar irradiance observations are made at the  $21^{st}$  of each month at noon. Depending on the number of days in the month, this date corresponds to 68% (for months with 31 days), 70% (for months with 30 days), or 75% (for February) of the month. The leap years are not considered and the  $21^{st}$  of February always corresponds to 75% of this month.

# Ambient Data Interpolation

The temperature is the only variable for which hourly data are available in addition to monthly averages. So for the temperature a double interpolation is performed to get a temperature profile for every time in a year depending on the date and the hour. For other data the interpolation is based on date only. This interpolation provides:

- The annual fluctuation of the dew-point temperature, the relative humidity, the wind speed, and the direct and diffuse solar irradiances
- The annual and diurnal fluctuation of the temperature

In all cases, the interpolation is of second order, with continuous first-order derivative.

### Ambient Variables and Conditions

The observed values are processed by computing weighted means, standard deviations, maximum, and minimum, to define different conditions for the temperature, dew-point temperature, and wind speed.

#### CONDITIONS OF TEMPERATURE

• Average:

$$T_{\rm amb} = \langle T_{\rm station} \rangle$$

• Low:

$$T_{\rm amb} = \langle T_{\rm station} \rangle - \sigma_{T, \, \rm station}$$

High:

$$T_{\text{amb}} = \langle T_{\text{station}} \rangle + \sigma_{T, \text{ station}}$$

• Lowest:

$$T_{\rm amb} = \min(T_{\rm station})$$

• Highest:

$$T_{\rm amb} = \max(T_{\rm station})$$

User defined coefficient for deviation:

$$T_{\text{amb}} = \langle T_{\text{station}} \rangle + c_{\sigma} \cdot \sigma_{T, \text{ station}}$$

• User defined correction:

$$T_{\rm amb} = \langle T_{\rm station} \rangle + \Delta T$$

where:

- $\langle T_{\rm station} \rangle$  (SI unit: K) is the weighted mean of the observed values of temperature at the station.
- σ<sub>T,station</sub> (SI unit: K) is the standard deviation of the observed values of temperature at the station.
- $T_{\text{station}}$  (SI unit: K) is the set of the observed values of temperature at the station.
- $c_{\sigma}$  (dimensionless) is a user-defined multiplicative coefficient applied to  $\sigma_{T, {
  m station}}$ .
- $\Delta T$  (SI unit: K) is a user-defined additive correction applied to  $\langle T_{\mathrm{station}} \rangle$ .

All these conditions are illustrated in Figure 2-3 for the variation of temperature over 1 day at New York/John F. Ke., on the 1<sup>st</sup> of June.

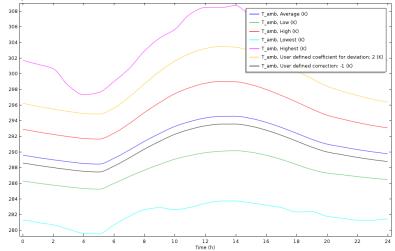


Figure 2-3: Comparison of ambient conditions for the temperature at New York/John F. Ke., on the 1st of June, with ASHRAE Weather Data Viewer 5.0 (©2013 ASHRAE, www.ashrae.org. Used with permission.).

Additional conditions are defined from observed couples of temperature and wind speed and direction values:

• Heating wind correlation:

$$T_{
m amb} = \langle T_{
m station} \rangle + \Delta T_{
m wind}$$

• Cooling wind correlation:

$$T_{\rm amb} = \langle T_{\rm station} \rangle - \Delta T_{\rm wind}$$

Here,  $\Delta T_{
m wind}$  (SI unit: K) is an additive correction applied to  $\langle T_{
m station} \rangle$ , defined as

$$\Delta T_{\rm wind} {=} \ \frac{1}{2} {\rm max}(\Delta T_{\rm ws, \, station}, \Delta T_{\rm wd, \, station})$$

where  $\Delta T_{\mathrm{ws,station}}$  (SI unit: K) and  $\Delta T_{\mathrm{wd,station}}$  (SI unit: K) are, respectively, the maximal variations of observed values of temperature correlated with a set of wind speed and direction observed values.

The heating and cooling wind correlations are illustrated in Figure 2-4 for the variation of temperature over 1 day, at New York/John F. Ke., on the 1<sup>st</sup> of June.

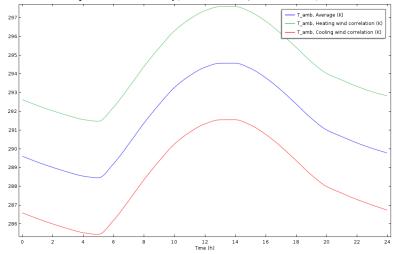


Figure 2-4: Comparison of heating and cooling wind correlations for the temperature at New York/John F. Ke., on the 1st of June, with ASHRAE Weather Data Viewer 5.0 (©2013 ASHRAE, www.ashrae.org. Used with permission.).

#### CONDITIONS OF DEW-POINT TEMPERATURE

• Average:

$$DPT_{amb} = \langle DPT_{station} \rangle$$

• Low:

$$DPT_{amb} = \langle DPT_{station} \rangle - \sigma_{DPT, station}$$

· High:

$$DPT_{amb} = \langle DPT_{station} \rangle + \sigma_{DPT, station}$$

• Lowest:

$$DPT_{amb} = min(DPT_{station})$$

• Highest:

$$DPT_{amb} = max(DPT_{station})$$

where:

- $\langle DPT_{station} \rangle$  (SI unit: K) is the weighted mean of the observed values of dew-point temperature at the station.
- σ<sub>DPT.station</sub> (SI unit: K) is the standard deviation of the observed values of dew-point temperature at the station.
- DPT<sub>station</sub> (SI unit: K) is the set of the observed values of dew-point temperature at the station.

All these conditions are illustrated in Figure 2-5 for the variation of the dew-point temperature over 1 year at New York/John F. Ke.

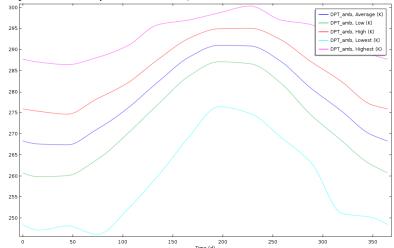


Figure 2-5: Comparison of the ambient conditions for the dew-point temperature at New York/John F. Ke., with ASHRAE Weather Data Viewer 5.0 (©2013 ASHRAE, www.ashrae.org. Used with permission.).

#### CONDITIONS OF WIND SPEED

• Average:

$$v_{\rm amb} = \langle v_{\rm station} \rangle$$

• Low:

$$v_{\rm amb} = \langle v_{\rm station} \rangle - \sigma_{v, \, \rm station}$$

• High:

$$v_{\rm amb} = \langle v_{\rm station} \rangle + \sigma_{v, \, \rm station}$$

• Lowest:

$$v_{\rm amb} = \min(v_{\rm station})$$

• Highest:

$$v_{\rm amb} = \max(v_{\rm station})$$

### where:

- $\langle v_{
  m station} 
  angle$  (SI unit: m/s) is the weighted mean of the observed values of wind velocity at the station.
- $\sigma_{v, \text{station}}$  (SI unit: m/s) is the standard deviation of the observed values of wind velocity at the station.
- $v_{\rm station}$  (SI unit: m/s) is the set of the observed values of wind velocity at the station.

All these conditions are illustrated in Figure 2-6 for the variation of the wind speed over 1 year at New York/John F. Ke.

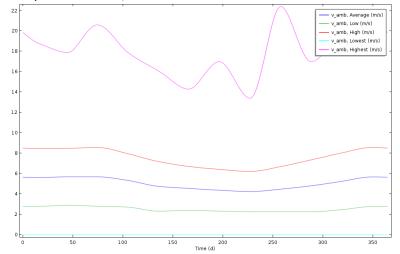


Figure 2-6: Comparison of the ambient conditions for the wind speed at New York/John F. Ke, with ASHRAE Weather Data Viewer 5.0 (©2013 ASHRAE, www.ashrae.org. Used with permission.).

#### CONDITIONS OF PRECIPITATION RATE

• Average:

$$P_{0, \text{ amb}} = \langle P_{0, \text{ station}} \rangle$$

• Low:

$$P_{0, \text{ amb}} = \langle P_{0, \text{ station}} \rangle - \sigma_{P_{0, \text{ station}}}$$

• High:

$$P_{0, \text{ amb}} = \langle P_{0, \text{ station}} \rangle + \sigma_{P_{0, \text{ station}}}$$

• Lowest:

$$P_{0, \text{ amb}} = \min(P_{0, \text{ station}})$$

• Highest:

$$P_{0, \text{ amb}} = \max(P_{0, \text{ station}})$$

Here:

- $\langle P_{0,\text{station}} \rangle$  (SI unit: m/s) is the weighted mean of the observed values of precipitation rate at the station.
- $\sigma_{P0,station}$  (SI unit: m/s) is the standard deviation of the observed values of precipitation rate at the station.
- $P_{0,\text{station}}$  (SI unit: m/s) is the set of the observed values of precipitation rate at the station.

#### PRESSURE

$$p_{\rm amb} = p_{\rm station}$$

where  $p_{\text{station}}$  (SI unit: Pa) is the observed value of absolute pressure at the station. Only a single value is available, so this data does not vary with time.

#### RELATIVE HUMIDITY

The relative humidity  $\phi_{amb}$  (dimensionless) is computed from the temperature  $T_{amb}$ and the dew-point temperature  $\ensuremath{\text{DPT}_{amb}}$  with the following relation:

$$\phi_{\rm amb} = \frac{p_{\rm sat}({\rm DPT_{amb}})}{p_{\rm sat}(T_{\rm amb})}$$

where  $p_{sat}(T_{amb})$  is the saturation pressure of vapor at  $T_{amb}$ 

As the diurnal variation of temperature is available, the diurnal fluctuations of relative humidity can be computed, as illustrated in Figure 2-7 for New York/John F. Ke, on the 1<sup>st</sup> of June, for different ambient conditions.

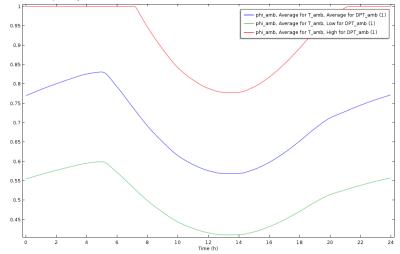


Figure 2-7: Diurnal fluctuations of relative humidity for different ambient conditions at New York/John F. Ke, on the 1st of June, with ASHRAE Weather Data Viewer 5.0 (©2013 ASHRAE, www.ashrae.org. Used with permission.).

Several conditions of relative humidity can be obtained from the selection of conditions for the temperature and dew-point temperature. For consistency, the relative humidity is majored by 1, as the red curve in Figure 2-7 shows.

### MOISTURE CONTENT

The moisture content  $x_{\text{vap,amb}}$  (dimensionless) is computed from the temperature  $T_{\rm amb}$ , the absolute pressure  $p_{\rm amb}$ , and the relative humidity  $\phi_{\rm amb}$  with the following relation:

$$x_{\rm vap,\,amb} = \frac{\phi_{\rm amb} \cdot p_{\rm sat}(T_{\rm amb})}{p_{\rm amb} - \phi_{\rm amb} \cdot p_{\rm sat}(T_{\rm amb})} \cdot \frac{M_{\rm v}}{M_{\rm a}}$$

where  $p_{\rm sat}(T_{\rm amb})$  is the saturation pressure of vapor at  $T_{\rm amb}$ , and  $M_{\rm v}$  and  $M_{\rm a}$  are the molar masses of water vapor and dry air

#### DIRECT AND DIFFUSE SOLAR IRRADIANCES

With clear sky conditions, the noon solar irradiance is essentially provided by the beam normal irradiance, coming directly from the sun. However, the diffuse horizontal

irradiance may be also considered. The sum of direct and diffuse solar irradiances is the ambient solar irradiance  $I_{s, amb}$  (SI unit: W/m<sup>3</sup>), defined by:

$$I_{s, amb} = I_{sn, station} + I_{sh, station}$$

where  $I_{\text{sn.station}}$  (SI unit: W/m<sup>3</sup>) and  $I_{\text{sh.station}}$  (SI unit: W/m<sup>3</sup>) are respectively the observed values of the clear sky noon beam normal and horizontal diffuse solar irradiances.

Figure 2-8 illustrates the evolution of ambient solar irradiance for New York/John F. Ke, over the year.

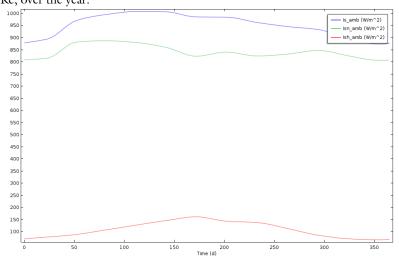


Figure 2-8: Decomposition of solar irradiance into normal and horizontal irradiance at New York/John F. Ke, with ASHRAE Weather Data Viewer 5.0 (©2013 ASHRAE, www.ashrae.org. Used with permission.).

# Use of Ambient Data From the Features

The ambient variables defined in the Ambient Properties node are available as inputs for several boundary and initial conditions. For example, when defining the heat transfer coefficient for a Heat Flux boundary condition by using a correlation for external forced

convection, the wind velocity  $v_{\rm amb}$ , the ambient absolute pressure  $p_{\rm amb}$ , and the ambient temperature  $T_{\rm amb}$  can be selected as inputs.

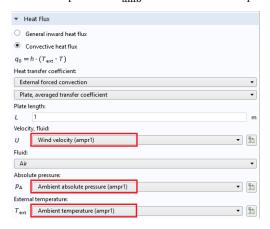


Figure 2-9: Use of ambient data from Heat Flux feature.

# 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
- The Phase Transport in Free and Porous Media Flow 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 ( $\Longrightarrow$ ) 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

The Laminar Flow (spf) interface (\infty) 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.

## Porous Treatment of No Slib Condition

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

#### Include Gravity

When the **Include gravity** 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 ( **a**) 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 estimate the influence of temporal variations in the velocity field, instead of using the inverse time step, in the consistent stabilization terms. This check box is selected by default

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

#### INCONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button ( **a**) 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**  $\delta_{id}$  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 ( **a** ) 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 check box under Linear solver 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
- 2 • 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 Source<sup>1</sup>
- Open Boundary
- Outlet

- Periodic Flow Condition
- Point Mass Source<sup>1</sup>
- Porous Interface
- Pressure Point Constraint
- Symmetry
- Volume Force
- Wall

<sup>&</sup>lt;sup>1</sup> A feature that may require an additional license



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

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



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

# Fluid Properties

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

#### MODEL INPUTS

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

#### Temperature

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

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

### Absolute Pressure

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

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

The default **Absolute pressure**  $p_A$  is  $p + p_{ref}$ , 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 ( **i** and entering the desired value in the input field.

2

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  $p_{\rm ref}$  for weakly compressible flows and  $p_{\rm ref}$  and  $T_{\rm ref}$  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**  $\mu$  describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

### Volume Force

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

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

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

# Initial Values

The initial values serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver in a stationary simulation. Note that for a transient compressible-flow simulation employing a material for which the density depends on the pressure (such as air), discontinuities in the initial values trigger pressure waves even when the Mach number is small. The pressure waves must be resolved and this puts a restriction on the time step.

#### INITIAL VALUES

Initial values or expressions should be specified for the **Velocity field u** and the **Pressure** p.

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

#### Wall

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

#### **BOUNDARY CONDITION**

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

No Slip

Leaking Wall

• Slip

No Slib

**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** is available when **Enable porous media domains** is activated in the **Physical Model** section in the settings for the main physics interface node. It specifies how **Wall** boundaries and **Interior Wall** boundaries adjacent to porous domains are treated. When **Standard no slip formulation** is chosen, a common no slip condition is applied on all solid walls. When the default **Porous slip** is chosen, a blending analytic expression is instead applied on the corresponding wall boundaries adjacent to the porous medium domain. It results in a no slip condition in case the porous length scale is fully resolved by the mesh and a slip condition in the

opposite limit when the mesh is much coarser than the porous scale. A smooth transition between these limits is ensured. Note that the interpretation and usage of nonzero slip at the wall is the same as in the **Navier slip** boundary condition. By default, **Velocity formulation** is on and the treatment is based on an approximate reconstruction of the far field pressure gradient using the slip velocity at the wall. If the Pressure-gradient formulation is chosen, the local pressure gradient at the wall is employed.

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<sub>tr</sub>. 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 uw 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 ( **a**) and selecting **Advanced Physics Options** in the **Show More Options** dialog box. The **Constraints** settings can be set to **Automatic**, **Pointwise constraints**, **Nitsche constraints**, or **Weak constraints**. **Mixed constraints** can be selected when imposing a no slip condition exactly.

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

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



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

#### Inlet

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

#### **BOUNDARY CONDITION**

The available Boundary condition options for an inlet are Velocity, Fully developed flow, 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  $p_{
    m ref}$ , 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 cleared by default to prescribe the total pressure pointwise. If it is selected, the averaged total pressure is imposed in the weak forms instead.

When Include gravity is selected and Use reduced pressure not selected in the interface Physical model section, the Compensate for hydrostatic pressure approximation (named Compensate for hydrostatic pressure for incompressible flows) 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  $\mathbf{d_u}$  (dimensionless) should be specified. The magnitude of  $\mathbf{d}_{\mathbf{n}}$  does not matter, only the direction.  $\mathbf{d}_{\mathbf{n}}$  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.

#### CONSTRAINT SETTINGS

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

Q	<ul><li> Prescribing Inlet and Outlet Conditions</li><li> Normal Stress Boundary Condition</li></ul>	
<b>Q</b>	Fully Developed Flow (Inlet)	

## 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 cleared, the total pressure is imposed pointwise.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface Physical model section, the Compensate for hydrostatic pressure approximation (named Compensate for hydrostatic pressure for incompressible flows) 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,  $P_{\mathrm{av}}$ . Observe that  $P_{\mathrm{av}}$  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.

### CONSTRAINT SETTINGS

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

<b>Q</b>	Prescribing Inlet and Outlet Conditions
<b>Q</b>	Fully Developed Flow (Outlet)

# Symmetry

This node provides a boundary condition for symmetry boundaries. It should only be used when the geometry and expected solution have mirror symmetry. By using

symmetries in a model its size can be reduced by one-half or more, making this an efficient tool for solving large problems.

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

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

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

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

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

### **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 ( **5** ) 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  $p \approx f_0$ .

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  $f_0$  user input.

No Viscous Stress

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

The **No viscous stress** condition prescribes:

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

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

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:

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

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

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  $p \approx f_0$ .

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  $f_0$  or  $p_{\text{hydro}}\mathbf{n}$  is added to  $\mathbf{F}$  depending of the selected option.

### CONSTRAINT SETTINGS

This section is displayed by clicking the **Show** button ( **a**) 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 (the **Destination Selection** section is optional). Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

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

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

#### **BOUNDARY SELECTION**



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

#### **DESTINATION SELECTION**

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

#### FLOW CONDITION

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

The **Flow Condition** at the boundary is specified through a value or expression for either the **Pressure difference**,  $p_{\rm src}$  –  $p_{\rm dst}$ , or the **Mass flow**,  $\dot{m}$  . The mass flow option ensures

a pressure difference is achieved across the source and destination boundaries. This pressure difference can, for example, drive the fully developed flow in a channel.

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

### ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( 5 ) and select **Advanced** Physics Options in the Show More Options dialog box. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the COMSOL Multiphysics Reference Manual.

# ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation** of Source section is changed from the default value, Automatic, and Advanced Physics **Options** is selected in the **Show More Options** dialog box. For information about the Orientation of Destination section, see Orientation of Source and Destination in the COMSOL Multiphysics Reference Manual.

### MAPPING BETWEEN SOURCE AND DESTINATION

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

# Porous Interface

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

Velocity and stress — stress continuity is invoked;

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

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

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

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

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

Vena contracta model allows two options:

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

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

# Flow Continuity

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

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

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

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# 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  $p_{\text{ref}}$  defined at the physics interface level is equal to zero,  $p_0$  represents the absolute pressure.

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

#### CONSTRAINT SETTINGS

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

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

### Point Mass Source

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

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

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

### SOURCE STRENGTH

The source Mass flux,  $\dot{q}_{\rm p}$  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.

### **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
- Porous Interface
- · Mass Sources for Fluid Flow
- Numerical Stability Stabilization Techniques for Fluid Flow
- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- Nitsche Constraints
- Particle Tracing in Fluid Flow
- References for the Single-Phase Flow, Laminar Flow Interfaces



The theory about most boundary conditions is found in Ref. 2.

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)

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

where

- $\rho$  is the density (SI unit: kg/m<sup>3</sup>)
- **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:  $N/m^3$ )
- $C_{\rm p}$  is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- T is the absolute temperature (SI unit: K)
- $\mathbf{q}$  is the heat flux vector (SI unit: W/m<sup>2</sup>)
- Q contains the heat sources (SI unit: W/m<sup>3</sup>)
- **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:

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

The dynamic viscosity,  $\mu$  (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  $\phi$ -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  $\phi$ -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  $\alpha$  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,  $\rho$  is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant p, 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  $\mathrm{Re}^c = \rho |\mathbf{u}| h/(2\mu)$  using the element length h for L and the magnitude of the velocity vector u for the velocity scale U. This Reynolds number is not related to the character of the flow field, but to the stability of the numerical discretization. The risk for numerical oscillations in the solution increases as  $\mathrm{Re}^c$  grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as:  $\mathrm{spf.cellRe}$ ).

#### DEFINITION

The gravity force is defined from the acceleration of gravity vector, **g**, and the density,  $\rho$ . 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  $\rho_{ref}$ , and assuming that  $\mathbf{g}$  is homogeneous, this equation is equivalently written:

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

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,  $\tilde{p} = p - \rho_{ref} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref})$ 

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

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

### 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  $p_A = p_{ref} + p$ . 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  $p_{\text{ref}}$ ,  $\mathbf{g}$ , and  $\mathbf{r}_0$  are defined consistently.

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

#### PRESSURE BOUNDARY CONDITION

For an immobile fluid the momentum equation simplifies to  $\nabla \cdot (p\mathbf{I}) = \mathbf{F} + \rho \mathbf{g}$  or

For incompressible flow, assuming there are no external forces, this leads respectively

to  $p = -\rho_{\text{ref}} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) + p_0 \text{ or } \tilde{p} = p_0$ .

 $\nabla \cdot (-\tilde{p}\mathbf{I}) = \mathbf{F} + (\rho - \rho_{ref})\mathbf{g}$  depending on the pressure formulation.

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 a special treatment of Wall boundaries and Interior Wall boundaries adjacent to porous domains (Porous Medium feature). Namely, similar to the Navier slip boundary condition, no penetration and tangential stress conditions are applied at the wall:

$$\begin{split} &\mathbf{u}\cdot\mathbf{n} \,=\, 0, \qquad \mathbf{K}_{\mathrm{n}} - (\mathbf{K}_{\mathrm{n}}\cdot\mathbf{n})\mathbf{n} \,=\, -\frac{\mu}{\epsilon_{\mathrm{p}}} \, \frac{\mathbf{u}_{\mathrm{slip}}}{y_{\mathrm{ps}}}, \\ &\mathbf{u}_{\mathrm{slip}} \!=\, \mathbf{u} - (\mathbf{u}\cdot\mathbf{n})\mathbf{n}, \qquad \mathbf{K}_{\mathrm{n}} \,=\, \frac{\mu}{\epsilon_{\mathrm{p}}} \, (\nabla\mathbf{u} \,+\! (\nabla\mathbf{u})^{\mathrm{T}})\mathbf{n} \end{split}$$

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

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

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

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

#### SLIDING WALL

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

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

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

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

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

- Automatic (default) use different constraint methods depending on whether only the normal component of the velocity is prescribed, such as in the no penetration condition,  $\mathbf{u} \cdot \mathbf{n} = 0$ , imposed, for example, in Slip walls or No Slip walls using Wall Functions or Automatic Wall Treatment, or both tangential and normal components are prescribed, as is the case of No Slip walls in laminar flow.
  - Nitsche constraints are used to impose the no penetration condition for Slip walls. When a No Slip condition is prescribed, pointwise constraints are used except for moving walls where Nitsche constraints are used.
- Pointwise constraints.
- Nitsche constraints.
- Weak constraints. They are not available on Interior Walls.
- Mixed constraints. This option is only available when both the tangential and normal components of the velocity need to be prescribed. The velocity on the wall normal direction is imposed via pointwise constraints. The constraint for the tangential directions is relaxed, and Nitsche constraints are used instead. This provides improved accuracy and performance when working with coarse boundary layer meshes. For more information, see Ref. 18.

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 permits specifying a complete velocity field at an outlet. This can, however, be difficult to apply in practice. The reason being that it is hard to prescribe the outlet velocity so that it is consistent with the interior solution at each point. The adjustment to the specified velocity then occurs across an outlet boundary layer. The thickness of this boundary layer depends on the Reynolds number; the higher the Reynolds number, the thinner the boundary layer.

#### ALTERNATIVE FORMULATIONS

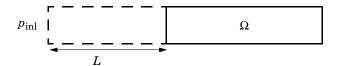
COMSOL provides several specialized boundary conditions that either provide detailed control over the flow at the boundary or that simulate specific devices. In practice they often prescribe a velocity or a pressure but calculate the prescribed values using, for example, ODEs.



Normal Stress Boundary Condition

# Fully Developed Flow (Inlet)

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



The flow to the domain  $\Omega$  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  $P_{\text{inl}}$  is applied on the inlet of the virtual channel.

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

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

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

$$\int_{\partial\Omega} \left( \left( L \left( -\mu (\nabla_{\mathbf{t}} \mathbf{u} + (\nabla_{\mathbf{t}} \mathbf{u})^{T}) + \frac{(p + P_{\text{inl}})}{2} \mathbf{I} \right) : (\nabla_{\mathbf{t}} \hat{\mathbf{u}}) \right) - P_{\text{inl}} (\mathbf{n} \cdot \hat{\mathbf{u}}) \right)$$

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

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

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

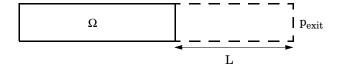
where <-> denotes the average over the inlet. Since the equation for  $P_{\rm inl}$  is a DAE (the equation for  $P_{\rm inl}$  does not contain  $P_{\rm inl}$ ), it must be solved coupled to Navier–Stokes and it must be treated by a Vanka presmoother and postsmoother if iterative solvers are used.

The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the inlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries). So in the figure above, if the lower boundary of  $\Omega$  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  $\Omega$  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  $P_{\text{exit}}$  is applied on the inlet of the virtual channel.

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

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

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

$$\int_{\partial\Omega} \left( \left( L \left( -\mu (\nabla_{\mathbf{t}} \mathbf{u} + (\nabla_{\mathbf{t}} \mathbf{u})^{T}) + \frac{(p + P_{\text{exit}})}{2} \mathbf{I} \right) : (\nabla_{\mathbf{t}} \hat{\mathbf{u}}) \right) - P_{\text{exit}} (\mathbf{n} \cdot \hat{\mathbf{u}}) \right)$$

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

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

equation (DAE) for  $P_{\rm exit}$ . 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  $P_{\rm ext}$  is a DAE, it must be solved coupled to Navier–Stokes and it must be treated by a Vanka presmoother and postsmoother if iterative solvers are used.

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

### No Viscous Stress

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

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

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

using the compressible/weakly compressible and the incompressible formulation, respectively.

The condition is not a sufficient outlet condition since it lacks information about the outlet pressure. It must hence be combined with pressure point constraints on one or several points or lines surrounding the outlet.

This boundary condition is numerically the least stable outlet condition, but can still be beneficial if the outlet pressure is nonconstant due to, for example, a nonlinear volume force.

# Normal Stress Boundary Condition

The total stress on the boundary is set equal to a stress vector of magnitude  $f_0$ , oriented in the negative normal direction:

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

$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = -f_0\mathbf{n}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This implies that the total stress in the tangential direction is zero. This boundary condition implicitly sets a constraint on the pressure which for 2D flows is

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

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

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

$$\begin{split} &\left(-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0\mathbf{n} \\ & (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -\hat{p}_0\mathbf{n} \\ & \hat{p}_0 \le p_0 \end{split} \tag{3-20}$$

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.

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

The ">" option is used with suppress backflow to have  $\mathbf{u} \cdot \mathbf{n} \le 0$  or  $\mathbf{u} \cdot \mathbf{r_u} \ge 0$ .

For incompressible single-phase flow, it is also allowed to specify the total pressure,  $p_{
m tot}$ , instead of the static pressure,  $p_{
m stat}$ , 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,  $p_{\text{stat}}$  is prescribed by:

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

where  $p_{\text{tot}}$  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.

# Porous Interface

This condition properly accounts for a sudden jump in porosity  $\varepsilon_{p}$  across boundary between different domains, giving the corresponding jump in stress across the interface. The emergence of a boundary layer on the upstream side of the interface is also revealed, which provides modifications to the behavior of the tangential velocity near the interface. The feature helps to avoid the need to add a very thin transition region, in which  $\varepsilon_{p,upstream}$  changes to  $\varepsilon_{p,downstream}$  continuously, while solving the Brinkman equation in such situations. Below, '-' and '+' (used as subscripts and superscripts) refer to the upstream and downstream side of the interface, respectively.

Whatever the option for **Continuity conditions** is chosen, the velocity conditions are

$$[\rho(\mathbf{u}\cdot\mathbf{n})]_{-}^{+}=0, \qquad \mathbf{u}_{t}|_{-}^{+}\equiv [\mathbf{u}-(\mathbf{u}\cdot\mathbf{n})\mathbf{n}]|_{-}^{+}=0$$

That is, the mass flux and tangential velocity across the interface are constant, and  $\mathbf{n}$  is assumed to be a normal pointing from '-' to '+'. Velocity and stress option just imposes usual stress continuity adding a correction for a possible jump in density:

$$\left[p\mathbf{n} - \mathbf{K}\mathbf{n} + \rho(\mathbf{u} \cdot \mathbf{n}) \left( \left[ \frac{1}{\varepsilon_{p}} \right]_{av}^{2} \mathbf{u} \right] \right]_{-}^{+} = 0$$

The option Velocity and porosity-corrected stress (default) adds a contribution due to the inertial term, which is non-trivial (gives non-zero effect) when  $\varepsilon_{\rm p}$  jumps across the interface:

$$\left[ p \mathbf{n} - \mathbf{K} \mathbf{n} + \rho (\mathbf{u} \cdot \mathbf{n}) \left( \left[ \frac{1}{\varepsilon_{p}} \right]_{av} \right)^{2} \mathbf{u} + \rho (\mathbf{u} \cdot \mathbf{n}) \left( \frac{1}{2\varepsilon_{p}^{2}} \right) \mathbf{u}_{av} \right] \right|^{+} = 0$$

Notice that 
$$\left[\frac{1}{\epsilon_p}\right]_{av} = \left(\left[\frac{1}{\epsilon_p}\right]_+ + \left[\frac{1}{\epsilon_p}\right]_+\right)/2$$
,  $\mathbf{u}_{av} = (\mathbf{u}_+ + \mathbf{u}_+)/2$  and so on.

Then, the Velocity and porosity-corrected stress with loss option has a 'pressure loss' term:

$$\left[p\mathbf{n} - \mathbf{K}\mathbf{n} + \rho(\mathbf{u} \cdot \mathbf{n}) \left(\left[\frac{1}{\varepsilon_{p}}\right]_{av}\right)^{2} \mathbf{u} + \rho(\mathbf{u} \cdot \mathbf{n}) \left(\frac{1}{2\varepsilon_{p}^{2}}\right) \mathbf{u}_{av}\right]\right|_{-}^{+} + p^{(loss)} \mathbf{n} = 0$$

This loss occurs in the downstream direction. Its mechanism is similar to the mechanism of common engineering 'total pressure loss'. Indeed, 'expansion' and 'contraction' across the interface experienced by the flow on the microscopic level (due to increasing or decreasing porosity,  $\varepsilon_p$ , respectively), are roughly equivalent to expansion and contraction of flow in a pipe with geometrical variations. Accordingly, it is assumed that only the normal velocity component is responsible for the loss. In the case of normal flow and negligible viscous term the pipe-analogy is quite exact.

Subsequently, Pressure loss model should be specified. Choosing User-defined loss coefficients requires values of Expansion loss coefficient and Contraction loss coefficient  $(K_{exp} = 1 \text{ and } K_{contr} = 0.5 \text{ are default values})$ . The resulting losses on the 'expansion' and 'contraction' boundaries are:

$$p^{(\text{loss,expansion})} = K_{\text{exp}} \left( \left( \frac{\rho(\mathbf{u} \cdot \mathbf{n})^2}{2\varepsilon_p^2} \right) \right),$$
$$p^{(\text{loss,contraction})} = K_{\text{contr}} \left( \frac{\rho(\mathbf{u} \cdot \mathbf{n})^2}{2\varepsilon_p^2} \right)_{\perp}$$

**Borda–Carnot** option results in the following losses:

$$p^{(\text{loss,expansion})} = \frac{\rho_{\text{av}}}{2} \left( \left[ \frac{(\mathbf{u} \cdot \mathbf{n})}{\varepsilon_{\text{p}}} \right]_{+} - \left[ \frac{(\mathbf{u} \cdot \mathbf{n})}{\varepsilon_{\text{p}}} \right]_{-} \right)^{2},$$

$$p^{(\text{loss,contraction})} = \frac{1}{2} \left( \frac{\rho(\mathbf{u} \cdot \mathbf{n})^{2}}{\varepsilon_{\text{p}}^{2}} \right)_{+} \left( \frac{1}{c_{\text{vc}}} - 1 \right)^{2}$$

and requires to choose **Vena contracta model**. The **User defined** option asks for value of **Vena contracta coefficient** ( $c_{vc} = 0.5$  by default). **Weisbach** option computes the coefficient based on the ratio of porosities across the interface:

$$c_{\text{vc}} = c_{\text{vc,ll}} + (1 - c_{\text{vc,ll}}) \left(\frac{\varepsilon_{\text{p,+}}}{\varepsilon_{\text{p,-}}}\right)^{n_{\text{vc}}}$$

and requires inputs for **Lower limit** and **Exponent** ( $c_{vc,ll} = 0.63$  and  $n_{vc} = 3$  are default values).

Although the velocity conditions formally look the same for all **Continuity conditions** options, the latter two (containing the inertial correction due to the porosity jump) lead to an extra non-trivial effect. Namely, the tangential velocity exponentially evolves over a boundary layer formed on the upstream side of the interface boundary. This boundary layer has a characteristic length equal to

$$l_{-} = \frac{\mu \varepsilon_{p,-}}{\rho(\mathbf{u} \cdot \mathbf{n})}$$

The ratio of the tangential velocities right after the interface ('downstream') and outside the boundary layer ('upstream infinity') is

$$\frac{\left|\boldsymbol{u}_{t,+}\right|}{\left|\boldsymbol{u}_{t,upstream\ infinity}\right|} = \frac{2\epsilon_{p,+}/\epsilon_{p,-}}{\epsilon_{p,+}/\epsilon_{p,-}+\epsilon_{p,-}/\epsilon_{p,+}}$$

In terms of the interstitial velocity,  $\mathbf{u}^{(i)} = \mathbf{u}/\varepsilon_{p}$ , this results in:

$$\frac{\left|\mathbf{u}^{(i)}_{t,+}\right|}{\left|\mathbf{u}^{(i)}_{t,upstream\ infinity}\right|} = \frac{2}{\epsilon_{p,+}/\epsilon_{p,-} + \epsilon_{p,-}/\epsilon_{p,+}} \leq 1$$

Obviously, tangential component of the interstitial kinetic energy is lost across the interface. For low viscosity and high normal-flow component, when  $l_u$  is much lower than  $l_{geom}$  (the characteristic geometry length) there are apparent variations in  $\mathbf{u}_t$  and  $\mathbf{u}^{(i)}$  in a thin boundary layer on the upstream side of the interface. However, for the cases with high viscosity or nearly interface-parallel flow,  $l_u$  is much larger than  $l_{geom}$ , and any variations in  $\mathbf{u}_t$  and  $\mathbf{u}^{(i)}_t$  are virtually invisible.

Notice that the feature does not take into account possible underresolved porous scale, as is described in Theory for the Free and Porous Media Flow, Darcy Interface.

# Mass Sources for Fluid Flow

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



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

#### POINT SOURCE

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

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

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,  $\dot{Q}$  must tend to plus or minus infinity as  $\delta V$  tends to zero. This means that in theory the pressure also tends to plus or minus infinity.

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

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

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

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

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

is added to lines in 3D or to points in 2D (which represent cut-through views of lines). Line sources can also be added to the axisymmetry line in 2D axisymmetry

components. It cannot, however, be added to geometrical lines in 2D because they represent physical planes.

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

2

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 ( **a** ) 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.

Streamline diffusion is active by default because it is necessary when convection is dominating the flow.

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

### CROSSWIND DIFFUSION

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

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

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

### STABILIZATION TIME SCALES

The time-scale tensor for time-dependent problems should in theory depend on a time-scale that many references just set to the time-step taken by the time-solver,  $\Delta t$ (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  $\Delta t^2$  in the time-scale tensor with measures of type  $(1/(\tilde{\Delta t})^2)^{-1}$ , 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** is activated.

The Limit small time steps effect on stabilization time scale option can be used to ramp down the time-step contribution in the stabilization when the time step becomes much smaller than the convective and diffusive time scales. This option prevents loss of pressure stabilization at such small time steps.

#### ISOTROPIC DIFFUSION

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



Numerical Stabilization and Iterative in the COMSOL Multiphysics Reference Manual

# Solvers for Laminar Flow

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

### NONLINEAR SOLVER

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

# Stationary Solver

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

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

#### Time-Dependent Solver

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

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

#### LINEAR SOLVER

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

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

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

Multigrid methods need smoothers, but the saddle point character of the linear system restricts the number of applicable smoothers. The choices are further restricted by the anisotropic meshes frequently encountered in fluid-flow problems. The efficiency of the smoothers is highly dependent on the numerical stabilization. Iterative solvers

perform at their best when both Streamline Diffusion and Crosswind Diffusion are active.

The default smoother for P1+P1 elements is SCGS. This is an efficient and robust smoother specially designed to solve saddle point systems on meshes that contain anisotropic elements. The SCGS smoother works well even without crosswind diffusion. SCGS can sometimes work for higher-order elements, especially if **Method** in the SCGS settings is set to **Mesh element lines**. But there is no guarantee for this, so the default smoother for higher order elements is an SOR Line smoother. SOR Line handles mesh anisotropy but does not formally address the saddle point character. It does, however, function in practice provided that streamline diffusion and crosswind diffusion are both active.

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

#### TIME-DEPENDENT SOLVERS

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

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

Both BDF and generalized- $\alpha$  are per default set to automatically adjust the time step. While this works well for many models, extra efficiency and accuracy can often be

gained by specifying a maximum time step. It is also often beneficial to specify an initial time step to make the solver progress smoothly in the beginning of the time series.

In the COMSOL Multiphysics Reference Manual:

2

- 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:

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

where  $\Delta \tilde{t}$  is a pseudo time step. Since **u**-nojac(**u**) is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a step of size  $\Delta \tilde{t}$  of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step  $\Delta t$  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<sub>loc</sub> 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<sub>loc</sub> 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<sub>loc</sub> 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<sub>loc</sub> too slowly or too quickly. CFL<sub>loc</sub> can then be tuned for the specific application.



For details about the CFL regulator, see Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual.

#### Nitsche Constraints

Some boundary conditions are implemented using Nitsche constraints. These boundary conditions include

- Wall Slip, sliding walls, and moving walls (that is, walls with nonzero translational velocity).
- · Periodic Flow Condition
- · Flow Continuity

The formulation used in the Fluid Flow interfaces in single-phase flow interfaces corresponds to the Symmetric Interior Penalty Galerkin method (SIPG). The SIPG method can be regarded to satisfy the boundary conditions in an integral sense rather than pointwise. More information on SIPG can be found in Ref. 15.

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

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 **x** is the position of the particle, m the particle mass, and **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

$$\operatorname{Re}_{p} = \frac{|\mathbf{u} - \mathbf{u}_{p}| 2r\rho}{u}$$

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

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

The model Flow Past a Cylinder (Application Library path

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**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 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 the Multiphysics Interfaces and Couplings chapter.
- 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 Layered Darcy's Law Interface describes low-velocity flow of fluids in layered materials (like layered soils, paperboard, composites, and so on) represented by boundaries. It is only available in 3D models and is only active on those boundaries where a layered material is defined.
- The Brinkman Equations Interface is intended for porous media high-velocity flows.

- The Free and Porous Media Flow, Brinkman Interface and The Free and Porous Media Flow, Darcy Interface combine 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.
- The Thin-Film and Porous Media Flow Interface couples the flow of a thin film of fluid described by Reynolds equation or modified Reynolds equation to low velocity flow in a porous medium governed by Darcy's law.

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:

- Theory for the Darcy's Law Interface
- 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
- Fracture Flow:
  - Theory for the Fracture Flow Interface
  - The Fracture Flow Interface
- Layered Darcy's Law:
  - Theory for the Layered Darcy's Law Interface
  - The Layered Darcy's Law Interface
- Brinkman Equations:
  - Theory for the Brinkman Equations Interface
  - The Brinkman Equations Interface

- Free and Porous Media Flow, Brinkman:
  - Theory for the Free and Porous Media Flow, Brinkman Interface
  - The Free and Porous Media Flow, Brinkman Interface
- Free and Porous Media Flow, Darcy:
  - Theory for the Free and Porous Media Flow, Darcy Interface
  - The Free and Porous Media Flow, Darcy 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 Models
- Average Linear Velocity
- Dual Porosity and Dual Permeability Theory
- References for the Darcy's Law Interface

# About Darcy's Law

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

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

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

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

# Darcy's Law — Equation Formulation

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

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

In this equation, **u** is the Darcy's velocity or specific discharge vector (SI unit: m/s);  $\kappa$  is the permeability of the porous medium (SI unit: m<sup>2</sup>);  $\mu$  is the fluid's dynamic viscosity (SI unit: Pa·s); p is the pore pressure (SI unit: Pa) and p is the density of the fluid (SI unit:  $kg/m^3$ ).

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



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

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

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

In the above equation,  $\rho$  is the fluid density (SI unit: kg/m<sup>3</sup>),  $\epsilon_p$  is the porosity, and  $Q_m$  is a mass source term (SI unit: kg/(m<sup>3</sup>·s)). Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

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

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

 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 Models

The continuity equation (Equation 4-2) allows flexible specification of relationships between parameters like density or permeability with respect to variables such as pressure, temperature, concentration, and more.

Expanding the time-derivative term and defining the porosity and density as functions of the pressure and using the chain rule results in

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

By inserting the definition of fluid compressibility  $\chi_f = (1/\rho)(\partial \rho/\partial p)$  to the right-hand side and rearrange the following expression is obtained

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

Using this relation, the generalized governing equation (Equation 4-2) takes the following form:

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

In this equation,  $S_p$  is the storage coefficient (SI unit: 1/Pa), which can be interpreted as the weighted compressibility of the porous material and the fluid. The storage can be an expression involving results from a solid-deformation equation or an expression involving temperatures and concentrations from other analyses. The Darcy's Law

interface implements Equation 4-4 in the Porous Medium node, which explicitly includes different storage models to choose from:

- From density and porosity, where the storage directly depends on changes in porosity or fluid density
- Linearized storage, which defines  $S_p$  using the compressibility of the fluid  $\chi_f$  and of the porous matrix  $\chi_p$  according to

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

Poroelastic storage where

$$S_{\rm p} = \varepsilon_{\rm p} \chi_{\rm f}$$
.



Storage models are only available for the Subsurface Flow Module and the Porous Media Flow Module. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

# Average Linear Velocity

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

# Dual Porosity and Dual Permeability Theory

The first well known publication on this topic is "The Behavior of Naturally Fractured Reservoirs" by J.E.Warren and P.J. Root from 1963. Since then the researchers further developed the idea of a dual porosity/permeability type of a porous medium. One of the well established models is based on the findings of H. Gerke and M. van Genuchten (Ref. 9). Basically the idea behind is to solve for each part of the porous medium (macro- and micropores) the relevant equations and connect them via an exchange term.

#### DUAL POROSITY MEDIUM

Darcy's Law is solved for the macropores and taking into account their volume fraction  $\theta_{\rm M}$  the equation reads:

$$\theta_{M} \left( \rho S_{p,M} \frac{\partial p_{M}}{\partial t} + \nabla (\rho \mathbf{u}_{M}) \right) = \theta_{M} Q_{M} - Q_{ip}$$
(4-5)

The term  $Q_{
m ip}$  describes the mass source from the Interporosity Flow which is the mass transfer from the macropores to the micropores system. An additional ODE for the (passive) micropores is solved which only act as additional storage volume:

$$(1 - \theta_M) \left( \rho S_{p,m} \frac{\partial p_m}{\partial t} \right) = (1 - \theta_M) Q_M + Q_{ip}.$$

The indices M and m stand for macropores and micropores, respectively.

#### **DUAL PERMEABILITY MEDIUM**

Darcy's law has to be solved for both the macroscale system and the microscale system:

$$\begin{split} \theta_{\mathrm{M}} & \left( \frac{\partial}{\partial t} (\varepsilon_{\mathrm{p,M}} \rho) + \nabla \cdot (\rho \mathbf{u}_{\mathrm{M}}) \right) = -Q_{\mathrm{ip}} + \theta_{\mathrm{M}} Q_{\mathrm{m}} \\ & (1 - \theta_{\mathrm{M}}) \left( \frac{\partial}{\partial t} (\varepsilon_{\mathrm{p,m}} \rho) + \nabla \cdot (\rho \mathbf{u}_{\mathrm{m}}) \right) = Q_{\mathrm{ip}} + (1 - \theta_{\mathrm{M}}) Q_{\mathrm{m}} \\ & p = \theta_{\mathrm{M}} p_{\mathrm{M}} + (1 - \theta_{\mathrm{M}}) p_{\mathrm{m}} \end{split} \tag{4-6}$$

 $\theta_{\mathrm{M}}$  is the volume fraction of the macropores,  $Q_{\mathrm{ip}}$  denotes the interporosity flow, signifying the mass transfer from the macropores (identified by index M) to the micropores (identified by index m).

Solving Darcy's law for both systems entails solving two equations, each associated with dependent pressure variables  $p_{\rm m}$  and  $p_{\rm M}$ . These equations are coupled via  $Q_{\rm in}$ . From this, average quantities for the dual permeability medium as a whole are computed. The average pressure of the dual permeability medium is defined as:

$$p = \theta_{\rm M} p_{\rm M} + (1 - \theta_{\rm M}) p_m$$

Likewise, average values for permeability, storage, velocity and other relevant parameters are computed.

#### UNSATURATED DUAL PERMEABILITY MEDIUM

Use the **Unsaturated Dual Permeability Medium** feature to model the transport in an unsaturated dual permeability medium where the Richards' Equation (Equation 4-26) describes the transport in each system.

$$\begin{split} \theta_{\mathrm{M}} \Big( \rho \Big( \boldsymbol{S}_{\mathrm{c},\mathrm{M}} \boldsymbol{S}_{\mathrm{p},\mathrm{M}} + \frac{\boldsymbol{C}_{\mathrm{m},\mathrm{M}}}{\rho g} \Big) \frac{\partial p_{\mathrm{M}}}{\partial t} + \nabla (\rho \mathbf{u}_{\mathrm{M}}) \Big) &= -\boldsymbol{Q}_{\mathrm{ip}} + \theta_{\mathrm{M}} \boldsymbol{Q}_{\mathrm{m}} \\ (1 - \theta_{\mathrm{M}}) \Big( \rho \Big( \boldsymbol{S}_{\mathrm{c},\mathrm{m}} \boldsymbol{S}_{\mathrm{p},\mathrm{m}} + \frac{\boldsymbol{C}_{\mathrm{m},\mathrm{m}}}{\rho g} \Big) \frac{\partial p_{\mathrm{m}}}{\partial t} + \nabla (\rho \mathbf{u}_{\mathrm{m}}) \Big) &= \boldsymbol{Q}_{\mathrm{ip}} + (1 - \theta_{\mathrm{M}}) \boldsymbol{Q}_{\mathrm{m}} \\ p &= \theta_{\mathrm{M}} p_{\mathrm{M}} + (1 - \theta_{\mathrm{M}}) p_{\mathrm{m}} \end{split} \tag{4-7}$$

 $\theta_{\mathrm{M}}$  is the volume fraction of the macropores,  $Q_{\mathrm{ip}}$  is the interporosity flow which is the mass transfer from the macroscale to the microscale system. The indices M and m stand for macropores and micropores, respectively.

#### INTERPOROSITY FLOW

Specify the **Fluid Transfer Function**  $\alpha_{\rm w}$  which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{\rm ip} = \alpha_{\rm w}(p_{\rm M} - p_{\rm m}) \tag{4-8}$$

with  $p_{\rm M}$  being the pressure within the macroscale system and  $p_{\rm m}$  the pressure within the microscale system

# References for the Darcy's Law Interface

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# The Darcy's Law Interface

The Darcy's Law (dl) interface ( No. ), 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 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 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.

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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 2 • 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 1111 • Steam Reformer: Application Library path Chemical\_Reaction\_Engineering\_Module/Reactors\_with\_Porous\_Catalysts/ steam\_reformer • Terzaghi Compaction: Application Library path Subsurface Flow Module/Poromechanics/terzaghi compaction

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

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

#### DOMAIN

- Porous Medium
- Unsaturated Porous Medium
- Dual Porosity Medium
- Dual Permeability Medium
- Unsaturated Dual Permeability Medium
- Mass Source
- Cross Section
- Initial Values
- · Unsaturated Porous Medium
- ThicknessContributing Velocity
- Porous Electrode Coupling

#### BOUNDARY, EDGE, AND POINT

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

- Atmosphere/Gauge
- Electrode Surface Coupling
- Flux Discontinuity
- Fracture
- Hydraulic Head
- Inlet
- Interior Wall
- Line Mass Source
- Mass Flux
- No Flow

- Outlet
- Pervious Layer
- Point Mass Source
- Precipitation
- Pressure
- Pressure Head
- Reaction Coefficients<sup>1</sup>
- Symmetry
- Thin Barrier

The relevant physics interface condition at interior boundaries is continuity:

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

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

<sup>&</sup>lt;sup>1</sup> 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

• Pervious Layer

· Pressure Head

• Flux Discontinuity

· Hydraulic Head

· Fracture

• Interior Wall

· Thin Barrier



Note that some of the above-mentioned domain or boundary conditions are only available with some products. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/



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



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



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

#### Porous Medium

The Porous Medium node adds the equations for modeling flow through porous domains. By default these are Equation 4-9 and Equation 4-10 (excluding any mass sources).

$$\frac{\partial}{\partial t}(\varepsilon_{p}\rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{m}$$
 (4-9)

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{4-10}$$

For a steady-state problem the first term in Equation 4-9 disappears. When Mass Source is active Equation 4-10 is of the following form:

$$\mathbf{u} = -\frac{\kappa}{\mu} (\nabla p - \rho \mathbf{g}) \tag{4-11}$$

The **Porous Medium** feature has two default subfeatures — the Fluid subfeature where the fluid density  $\rho$  (SI unit: kg/m<sup>3</sup>) and dynamic viscosity  $\mu$  (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability  $\kappa$  (SI unit:  $m^2$ ) and porosity  $\varepsilon_{\rm p}$  (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 4-9 and Equation 4-10.
- Non-Darcian flow defines a nonlinear relationship using Equation 4-9 and

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

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

### STORAGE MODEL

Define the time dependent storage term by selecting one of the following options from the drop-down menu:

• From density and porosity (default), uses the formulation of Equation 4-9

• Linearized storage, where the following linear equation is used to define the storage:

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

- **Poroelastic storage**, where  $S_p = \varepsilon_p \chi_f$
- Quasistatic, where the storage term is set to zero
- User defined to directly specify the storage coefficient  $S_{
  m p}$

<b>Q</b>	<ul> <li>Porous Material in the COMSOL Multiphysics Reference Manual</li> <li>About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide</li> <li>Storage Models in the Subsurface Flow Module User's Guide</li> </ul>
Q	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/

# Fluid

This node defines the material properties of the fluid of the Porous Medium, the Unsaturated Porous Medium, the Dual Porosity Medium, the Dual Permeability Medium, or the Unsaturated Porous Medium parent node.

#### MODEL INPUT

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

#### **FLUID PROPERTIES**

The available options for the Fluid type are Incompressible, Compressible, Compressible, linearized, or Ideal gas. The selection determines how the density and compressibility of the fluid are set.

#### Incompressible

The default Reference density  $\rho_{\rm ref}$  uses values From material. For User defined enter another value or expression.

#### Compressible

The default **Density**  $\rho$  uses values **From material**. For **User defined** enter another value or expression as a function of the absolute pressure. The compressibility of the fluid is computed from it.

#### Compressible, Linearized

The default Reference density  $\rho_{ref}$  and the Fluid compressibility  $\chi_f$  use values From material. For User defined enter another value or expression. The fluid density increases linearly as a function of the fluid pressure.

#### Ideal Gas

For **Ideal gas** it uses the ideal gas law to describe the gas density. In this case, specify the thermodynamics properties. Select a Gas constant type — Specific gas constant  $R_s$ (the default) or Mean molar mass  $M_n$  (SI unit:  $J/(\text{mol} \cdot K)$ ). 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.

For all fluid types specify the **Dynamic viscosity**  $\mu$  (SI unit: Pa·s) uses values **From** material. For User defined enter another value or expression.

#### 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:

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

where  $\theta_{si}$  and  $\theta_{imfi}$  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  $\chi_D = 10^{-4} \text{ l/Pa}$ .

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**  $d_p$  (SI unit: m), the default value is 0.5 mm.

#### Non-Darcian Flow

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

- For Forchheimer, the default Permeability  $\kappa(SI \text{ unit: m}^2)$  uses the value From material. Furthermore, the dimensionless Forchheimer parameter  $c_{\rm F}$  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  $\kappa_{\infty}$  (SI unit: m<sup>2</sup>) uses the value From material. Enter the Klinkenberg parameter  $b_K$ . Its default value is  $10^3~{\rm Pa}$ .

2	<ul> <li>About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide</li> <li>Permeability Models in the Porous Media Flow Module User's Guide</li> </ul>
<b>Q</b>	Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

#### RETENTION MODEL

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

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

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



The **Unsaturated Porous Medium** node adds the Richards' equation (Equation 4-12) for flow in variably saturated porous media.

$$\rho \left( \frac{C_{\rm m}}{\rho g} + S_{\rm e} S_{\rm p} \right) \frac{\partial p}{\partial t} + \nabla \cdot \rho \left( -\frac{\kappa_{\rm r} \kappa}{\mu} (\nabla p + \rho g \nabla D) \right) = Q_{\rm m}$$
 (4-12)

The Unsaturated Porous Medium feature has two default subfeatures: the Fluid subfeature, where the fluid density ρ (SI unit: kg/m<sup>3</sup>) and viscosity μ (SI unit: Pa·s) are defined, and the Porous Matrix subfeature, where the permeability  $\kappa$  (SI unit: m<sup>2</sup>) and porosity  $\varepsilon_{\rm p}$  (dimensionless) are specified as well as the retention model.

#### COORDINATE SYSTEM SELECTION

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

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

#### STORAGE MODEL

With this option, define the first term in Equation 4-12. Therefore, choose from a drop-down menu one of the following formulations:

- · From retention model
- Linearized storage (default)
- From liquid content
- User defined

If From retention model is chosen, the first term of Equation 4-12 accounts only for the specific moisture capacity  $C_{\rm m}$  which is defined by the Retention Model in the Porous Matrix subnode:

$$\frac{C_m}{g} \frac{\partial p}{\partial t}$$
.

For the option Linearized storage the storage coefficient  $S_{\rm p}$  in Equation 4-12 is defined as

$$S_{\rm p} = \varepsilon_{\rm p} \chi_{\rm f} + (1 - \varepsilon_{\rm p}) \chi_{\rm p}$$
.

From liquid content enforces the first term of Equation 4-12 to be defined in terms of liquid volume fraction as

$$\frac{\partial(\rho\theta_l)}{\partial t}$$

and the **User defined** option allows to define the storage coefficient  $S_p$  in Equation 4-12 directly.

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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/

# Dual Porosity Medium

Use the Dual Porosity Medium if the flow through macropores is governed by Darcy's law and the micropores do not significantly contribute to the overall flow in the porous medium.

The feature has three default subfeatures —the Fluid subfeature where the fluid density  $\rho$  (SI unit: kg/m<sup>3</sup>) and dynamic viscosity  $\mu$  (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

#### COORDINATE SYSTEM SELECTION

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

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

#### STORAGE MODEL

Choose from a drop-down menu one of the following formulations:

• From density and porosity (default), uses the formulation equivalent to Equation 4-9

- Linearized storage, where the following linear equation is used to define the storage in the macropores as  $S_p = \varepsilon_p \chi_f + (1 - \varepsilon_p) \chi_p$  and in the micropores as  $S_{p,m} = \varepsilon_{p,m} \chi_f + (1 - \varepsilon_{p,m}) \chi_p$ .
- Poroelastic storage, where  $S_p = \varepsilon_p \chi_f$  in the macropores and  $S_{p,m} = \varepsilon_{p,m} \chi_f$  in the micropores.
- Quasistatic, where the storage term is set to zero
- **User defined** to directly specify the storage coefficient  $S_{\rm p}$  and  $S_{\rm p,m}$  for the macroand micropores respectively.

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• Storage Models in the Subsurface Flow Module User's Guide

#### INTERPOROSITY FLOW

Specify the **Fluid Transfer Function**  $\alpha_{w}$  which is used to calculate the interporosity flow, the mass exchange between macro- and microscale system:

$$Q_{\rm ip} = \alpha_{\rm w}(p_{\rm M} - p_{\rm m}) \tag{4-13}$$

with  $p_{\rm M}$  being the pressure within the macropores and  $p_{\rm m}$  the pressure within the micropores.

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Find more information in the Subsurface Flow Module User's Guide

- Dual Porosity & Dual Permeability Modeling
- Dual Porosity and Dual Permeability Theory

2

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/

# Dual Permeability Medium

Use the Dual Permeability Medium feature to model transport in a saturated dual permeability medium where Darcy's Law describes the transport in each system.

The feature has three default subfeatures —the Fluid subfeature where the fluid density  $\rho$  (SI unit: kg/m<sup>3</sup>) and dynamic viscosity  $\mu$  (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

#### COORDINATE SYSTEM SELECTION

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

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

#### STORAGE MODEL

With this option under the **Porous Medium** section, Equation 4-9 is formulated with respect to a storage term (analogous to Equation 4-4). Therefore, choose from a drop-down menu one of the following formulations:

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

$$S_{p,i} = \varepsilon_{p,i} \chi_f + (1 - \varepsilon_{p,i}) \chi_{p,i}$$

with i=M for the macropores and i=m for the micropores.

- Poroelastic storage, where  $S_{\mathrm{p,i}}$  =  $\varepsilon_{\mathrm{p,i}}\chi_{\mathrm{f}}$
- Quasistatic, where the storage term is set to zero
- User defined to directly specify the storage coefficient  $S_{
  m p}$



• Storage Models in the Subsurface Flow Module User's Guide

#### INTERPOROSITY FLOW

Specify the **Fluid Transfer Function**  $\alpha_{\rm w}$  which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{\rm ip} = \alpha_{\rm w}(p_{\rm M} - p_{\rm m}) \tag{4-14}$$

with  $p_{\rm M}$  being the pressure in the macropores and  $p_{\rm m}$  the pressure in the micropores.

Find more information in the Subsurface Flow Module User's Guide 2 • Dual Porosity & Dual Permeability Modeling • Dual Porosity and Dual Permeability Theory

Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit 2 https://www.comsol.com/products/specifications/

# Unsaturated Dual Permeability Medium

Use the Unsaturated Dual Permeability Medium feature to model the transport in an unsaturated dual permeability medium where the Richards' Equation (Equation 4-12) describes the transport in each system.

$$\begin{split} \theta_{\mathrm{M}} \Big( \rho \Big( \boldsymbol{S}_{\mathrm{e},\mathrm{M}} \boldsymbol{S}_{\mathrm{p},\mathrm{M}} + \frac{\boldsymbol{C}_{\mathrm{m},\mathrm{M}}}{\rho g} \Big) \frac{\partial p_{\mathrm{M}}}{\partial t} + \nabla (\rho \mathbf{u}_{\mathrm{M}}) \Big) &= -\boldsymbol{Q}_{\mathrm{ip}} + \theta_{\mathrm{M}} \boldsymbol{Q}_{\mathrm{m}} \\ (1 - \theta_{\mathrm{M}}) \Big( \rho \Big( \boldsymbol{S}_{\mathrm{e},\mathrm{m}} \boldsymbol{S}_{\mathrm{p},\mathrm{m}} + \frac{\boldsymbol{C}_{\mathrm{m},\mathrm{m}}}{\rho g} \Big) \frac{\partial p_{\mathrm{m}}}{\partial t} + \nabla (\rho \mathbf{u}_{\mathrm{m}}) \Big) &= \boldsymbol{Q}_{\mathrm{ip}} + (1 - \theta_{\mathrm{M}}) \boldsymbol{Q}_{\mathrm{m}} \\ p &= \theta_{\mathrm{M}} p_{\mathrm{M}} + (1 - \theta_{\mathrm{M}}) p_{\mathrm{m}} \end{split} \tag{4-15}$$

 $\theta_{
m M}$  is the volume fraction of the macropores,  $Q_{
m ip}$  is the interporosity flow which is the mass transfer from the macroscale to the microscale system. The indices M and m stand for macropores and micropores, respectively.

The feature has three default subfeatures —the Fluid subfeature where the fluid density  $\rho$  (SI unit: kg/m<sup>3</sup>) and dynamic viscosity  $\mu$  (SI unit: Pa·s) are defined, the Macropores subfeature where the hydraulic properties of the macroporous matrix are defined, and the Micropores where the hydraulic properties of the microporous matrix are defined.

#### COORDINATE SYSTEM SELECTION

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

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

#### STORAGE MODEL

With this option, define the first term in Equation 4-15. Therefore, choose from a drop-down menu one of the following formulations:

- · From retention model
- Linearized storage (default)
- · From liquid content
- · User defined

If From retention model is chosen, the first term of Equation 4-15 accounts only for the specific moisture capacity  $C_{\mathrm{m,i}}$  which is defined by the Retention Model in the Macropores (i=M) or Micropores (i=m) subnode:

$$\frac{C_{\mathrm{m}i}\partial p}{g}$$
.

For the option **Linearized storage** the storage coefficient  $S_{p,i}$  in Equation 4-15 is defined as

$$S_{p,i} = \varepsilon_{p,i} \chi_f + (1 - \varepsilon_{p,i}) \chi_{p,i}$$
.

From liquid content enforces the first term of Equation 4-15 to be defined in terms of liquid volume fraction as

$$\frac{\partial (\rho \theta_{l,i})}{\partial t}$$

ullet and the **User defined** option allows to define the storage coefficient  $S_{
m p,i}$  in Equation 4-15 directly.

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• Storage Models in the Subsurface Flow Module User's Guide

#### INTERPOROSITY FLOW

Specify the **Fluid Transfer Function**  $\alpha_{\rm w}$  which is used to calculate the interporosity flow, which is the mass exchange between macro- and microscale system:

$$Q_{\rm ip} = \alpha_{\rm w}(p_{\rm M} - p_{\rm m}) \tag{4-16}$$

with  $p_{\rm M}$  being the pressure within the macroscale system and  $p_{\rm m}$  the pressure within the microscale system.

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• Dual Porosity & Dual Permeability Modeling in the Subsurface Flow Module User's Guide

# Macropores

This node defines the porosity and material properties of the macroporous matrix of the Dual Porosity Medium, the Dual Permeability Medium, or the Unsaturated Dual Permeability Medium parent node.

#### MODEL INPUT

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

#### **VOLUME FRACTION**

Here enter the Volume Fraction of Macropores,  $\theta_{M}$ .

#### MATRIX PROPERTIES

The default **Porosity**  $\varepsilon_{p,M}$  of the solid matrix of the macropore system is taken **From** material. Select User defined to enter a value or expression for  $\varepsilon_{n,M}$ .

If required by a Storage model in the parent node, specify the Effective compressibility of the porous matrix of the macropore system. The default value is  $\chi_{p,M} = 10^{-4} \text{ 1/Pa}$ .

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. For the macropore settings only the Darcian Flow models are available. Select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability**  $\kappa_{\rm M}$  (SI unit: m<sup>2</sup>) 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  $K_{\rm M}$  (SI unit: m/s) select Isotropic to

define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is  $2.94 \cdot 10^{-4}$  m/s.

• Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean Particle diameter  $d_{\rm p,M}$  (SI unit: m), the default value is 0.5 mm.

#### RETENTION MODEL

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

- van Genuchten, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants  $\alpha$  (the default value is 1, and the SI unit is 1/m), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to 1 - 1/n.
- Brooks and Corey to use the retention model according to the Brooks and Corey relationships.
- User defined to use a different retention model. Enter user defined expressions for the Effective saturation  $S_{e,M}$ , the Liquid volume fraction  $\theta_{l,M}$ . The default is  $\epsilon_{p,M}$  (the porosity variable). Specify the Specific moisture capacity  $C_{\mathrm{m,M}}$  (SI unit:  $1/\mathrm{m}$ ). The default value is 0 (1/m). Enter an expression for the **Relative permeability**  $\kappa_{r,M}$ . The default value is 1.

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



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

# Micropores

This node defines the porosity and material properties of the microporous matrix of the Dual Porosity Medium, Dual Permeability Medium, or the Unsaturated Dual Permeability Medium parent node.

#### MODEL INPUT

This section is only available for the Unsaturated Dual Permeability Medium parent node and contains fields and values that are inputs for expressions defining material

properties. If such user-defined property groups are added, the model inputs appear here.

## MATRIX PROPERTIES

The default **Porosity**  $\varepsilon_{p,m}$  of the solid matrix of the micropore system is taken **From** material. Select User defined to enter a value or expression for  $\varepsilon_{n,m}$ .

If required by a Storage model in the parent node, specify the Effective compressibility of the microscale porous matrix. The default value is  $\chi_{n,m} = 10^{-4} \text{ 1/Pa}$ .

Select a Permeability model to specify the capacity to transmit flow for the porous material of the microscale system. Here, only the Darcian Flow models are available. Select between the following options for the **Permeability model**:

- Select **Permeability** (default) to define the permeability of the porous matrix. The default **Permeability**  $\kappa_{\rm m}$  (SI unit: m<sup>2</sup>) 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  $K_{\rm m}$  (SI unit: m/s) select Isotropic to define a scalar value or Diagonal or Symmetric to define a tensor value. The default is  $2.94 \cdot 10^{-4}$  m/s.
- Select **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter. Enter the mean **Particle diameter**  $d_{p,m}$  (SI unit: m), the default value is 0.5 mm.

## RETENTION MODEL

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

- From macropores to take over the retention model settings from the Macropores node.
- van Genuchten, to specify the retention model using the van Genuchten relationship. Enter the constitutive relation constants  $\alpha$  (the default value is 1, and the SI unit is 1/m), n (default value is 2), and l (default value is 0.5). The constitutive parameter m is equal to 1 - 1/n.
- Brooks and Corey to use the retention model according to the Brooks and Corey relationships.
- User defined to use a different retention model. Enter user defined expressions for the Effective saturation  $S_{e,m}$ , the Liquid volume fraction  $\theta_{l,m}$ . The default is  $\varepsilon_{p,m}$  (the

porosity variable). Specify the **Specific moisture capacity**  $C_{m,m}$  (SI unit: 1/m). The default value is 0 (1/m). Enter an expression for the **Relative permeability**  $\kappa_{r,m}$ . The default value is 1.

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

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

## INITIAL VALUES

Define the initial pressure of the microscale system. The default is to use the initial values defined in the Initial Values feature node which means that the same initial values apply to the macroscale and the microscale system.

Select **User Defined** to specify an initial pressure for the microscale system  $p_{\rm m0,init}$ .



Note that some options are only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

# 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 4-9).

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_{\mathrm{m}}$$
 (4-17)

For the Fracture Flow interface, the mass source is applicable to the right-hand side of Equation 4-40 in the Subsurface Flow Module User's Guide or Equation 4-31 in the Porous Media Flow Module User's Guide (where it is multiplied with the fracture thickness).

## MASS SOURCE

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

The Contributing Velocity node adds a velocity contribution  $\mathbf{u}_{\mathrm{ctrb}}$  to the velocity field  $\mathbf{u}_{d}$  that is computed from the flow model selected in the parent Porous Medium, Unsaturated Porous Medium, or Dual Porosity Medium feature. The total velocity field used in the continuity equation is therefore

$$\mathbf{u} = \mathbf{u}_{d} + \mathbf{u}_{ctrb} \tag{4-18}$$

Such velocity contributions can arise in multiphysics models that involve, for example, transport of solutes. If several Contributing Velocity nodes are added under the same parent feature, the contributions are treated additively. The sum of all contributing velocity fields is available in the variables name. Uctrb (material frame) and name.uctrb (spatial frame), with name being the Name of the physics interface (for example, d1).

## COORDINATE SYSTEM SELECTION

Select a coordinate system from the Coordinate system list to specify the coordinate system in which the contributing velocity field is given. The default is the Global coordinate system. Note that the coordinate system used to specify the components of the contributing velocity field can be selected independently of the coordinate system of the parent feature.

## CONTRIBUTING VELOCITY

The default contributing velocity field  $u_{\text{ctrb}}$  is User defined, which lets you enter the components of the contributing velocity field explicitly. If a matching velocity field is announced by another feature, it will be available in the selection list.

## ADVANCED

Select the Frame in which the contributing velocity field is specified. The default is the **Reference configuration**, which means that the velocity field follows the material under, for example, a rotation of the domain. If instead your contributing velocity field follows a fixed direction in space, select the **Deformed configuration**. This section is only displayed if Advanced Physics Options is activated and the spatial and material frame of the component differ, such as in the presence of a Moving Mesh or Solid Mechanics interface.

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  $\rho$  is the fluid density (SI unit: kg/m<sup>3</sup>); 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  $H_n$  (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.

# Gravity

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

# COORDINATE SYSTEM SELECTION

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

## GRAVITY

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

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

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

When **Elevation** is selected from the list, specify the **Elevation** D (SI unit: m). The Acceleration of gravity is taken From physics interface by default but could be overridden when User defined is selected.

When the check box **Include gravity** is not selected in the Darcy's Law interface Settings, the elevation D is set equal to zero.

Select the check box **Specify reference position** to define a reference position for the gravity calculation.

# 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 (the z direction with default spatial coordinate names). In 1D axisymmetric geometries the thickness represents the z direction.

## THICKNESS

Specify a value for the  ${\it Thickness}\ d_z$  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.

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

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

## SPECIES

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

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

# Electrode Surface Coupling

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

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

## SPECIES

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

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

# Pressure

Use the **Pressure** node to specify the pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition  $p = p_0$  where  $p_0$  is a known pressure given as a number, a distribution, or an expression involving time, t, for example.

## PRESSURE

Enter a value or expression for the **Pressure**  $p_0$  (SI unit: Pa). Enter a relative pressure value in  $p_0$  (SI unit: Pa).

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

## CONSTRAINT SETTINGS

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

As an attribute to the Fracture boundary condition or as boundary condition to The Fracture Flow Interface (which are available in the Subsurface Flow Module and the Porous Media Flow Module), the pressure can also be specified on edges (in 3D) or points (in 2D) surrounding the fracture domain. In other cases, pressure constraints on edges or points are not implemented.



If the boundary condition is adjacent to an Unsaturated Dual Permeability Medium feature it constrains the pressures in the Macropores and Micropores to  $p_0$ .

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

# Line Mass Source

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

## SELECTION

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

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

## LINE MASS SOURCE

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

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

## Fracture Flow

The equivalent feature available for fracture flow is the Mass Source attribute of the Fracture boundary condition and the Mass Source point feature of the Fracture Flow Interface, both available in 3D only.

# 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.

# Inlet

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

## VELOCITY

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

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

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

#### PRESSURE

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

## MASS FLOW

If you select Mass flow as the inlet condition, specify the total Mass flow rate  $M_0$  (SI unit: kg/s), or the **Pointwise mass flux**  $N_0$  (SI unit: kg/(m<sup>2</sup>·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 ( **a**) 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.

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,  $\rho$  is the fluid density, **u**<sub>1</sub> and **u**<sub>2</sub> are the Darcy velocities in the adjacent domains (as defined in Equation 4-19) and  $N_0$  is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{4-19}$$

For this boundary condition, a positive value of  $N_0$  corresponds to a flow discontinuity in the opposite direction to the normal vector of the interior boundary.

## MASS FLUX

Enter a value or expression for the **Inward mass flux**  $N_0$  (SI unit: kg/(m<sup>2</sup>·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 unit: Pa).

## DISCHARGE

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

$$\int_{\partial\Omega} \rho \mathbf{u} \cdot \mathbf{ds} = \rho Q_D. \tag{4-20}$$

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

# 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.

# 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.

# Thin Barrier

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

## WALL

Enter a value or expression for the **Thickness**  $d_b$  (SI unit: m, the default is 0.1 m) and for the **Permeability**  $\kappa_b$  (SI unit: m<sup>2</sup>). The default **Permeability**  $\kappa_b$  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).

## 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 ( **a** ) 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.

## 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 ( **a**) 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.

## CONSTRAINT SETTINGS

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

# Pervious Layer

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

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = \rho R_{b} \left[ \frac{(p_{b} - p)}{\rho g} + (D_{b} - D) \right]$$
 (4-21)

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:

$$\mathbf{n} \cdot \rho K \nabla (H_p + D) = \rho R_b [(H_{pb} - H_p) + (D_b - D)]$$
 (4-22)

 $H_{\rm pb}$  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:

$$\mathbf{n} \cdot \rho K \nabla H = \rho R_{\mathbf{b}} [H_{\mathbf{b}} - H] \tag{4-23}$$

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

K in Equation 4-22 and Equation 4-23 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**  $R_b$  (SI unit: 1/s).

- For Pressure and elevation enter an External pressure  $p_b$  (SI unit: Pa) and External elevation  $D_{\mathbf{b}}$  (SI unit: m).
- For Pressure head and elevation enter an External pressure head  $H_{p\mathrm{b}}$  (SI unit: m),  $H_{p\mathrm{b}}$ (SI unit: m) and External elevation  $D_{\rm b}$  (SI unit: m).
- For Hydraulic head enter the Hydraulic head  $H_{\mathrm{b}}$  (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.

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:  $kg/(m^2 \cdot s)$ ).

Use the Fracture node to model flow along a boundaries representing fractures within a porous medium. By default, it adds the tangential form of the continuity equation and of Darcy's Law.

$$d_{f}\frac{\partial}{\partial t}(\varepsilon_{p}\rho) + \nabla_{T} \cdot (d_{f}\rho \mathbf{u}) = d_{f}Q_{m}$$
 (4-24)

$$\mathbf{u} = -\frac{\kappa}{\Pi} \nabla_{\mathrm{T}} p \tag{4-25}$$

The **Fracture** feature has two default subfeatures — the Fluid (Fracture) subfeature where the fluid density ρ (SI unit: kg/m<sup>3</sup>) and dynamic viscosity μ (SI unit: Pa·s) are defined and the Fracture Material subfeature where the permeability  $\kappa$  (SI unit:  $m^2$ ) and porosity  $\epsilon_{\!{}_{\rm p}}$  (dimensionless) are specified.

## COORDINATE SYSTEM SELECTION

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

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

## APERTURE

Enter a value for the **Fracture thickness**  $d_{\mathrm{f}}$ .

## FLOW MODEL

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

- Darcian flow (default) defines a linear relationship using Equation 4-24 and Equation 4-25.
- Non-Darcian flow defines a nonlinear relationship using Equation 4-24 and the pressure-velocity relationship

$$\nabla_{\mathrm{T}} p = -\frac{\mu}{\kappa} \mathbf{u} - \beta \rho |\mathbf{u}| \mathbf{u}$$

where the nonlinear parameter  $\beta$  (SI unit: 1/m) is further specified in the Fracture Material subfeature.

## STORAGE MODEL

Equation 4-24 can also be formulated with respect to a storage term.

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

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 4-24
- **Linearized storage**, where the following linear equation is used to define the storage:

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

• User defined to directly specify the storage coefficient S



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

# FRACTURE MODEL

Choose between two options to model fractures that have different characteristics.

- Highly conductive fracture represents a fracture filled with a highly permeable material.
- Thin conducting barrier represents a fracture that is filled with a low permeable material and therefore acts as a barrier for the flow which adds a jump in the pressure across the boundary:

$$-\mathbf{n}_{\mathrm{u,d}} \cdot (\rho \mathbf{u})_{\mathrm{u,d}} = \rho \frac{(p_{\mathrm{d,u}} - p_{\mathrm{u,d}}) \kappa_{\mathrm{b}}}{d_{\mathrm{b}}} \frac{\kappa_{\mathrm{b}}}{\mu}$$

The barrier thickness  $d_b$  and permeability  $\kappa_b$  are defined in the Fracture Material subnode.

In addition, either on the upside, downside, or on both sides a highly conductive fracture material is present and Equation 4-24 and Equation 4-25 are solved for the highly conductive side. Further specifications are done in the Fracture Material subnode.



Note that the option to specify the Fracture Model is only available for the Fracture feature within the Darcy's Law interface.

For the Fracture boundary node several subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. As they are almost identical to the boundary conditions of the Fracture Flow interface, see Domain, Boundary, Edge, Point, and Pair Nodes for the Fracture Flow Interface for further description. Note that **Precipitation** is only available for the Fracture Flow interface.



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



Flow in a Fractured Reservoir: Application Library path Subsurface\_Flow\_Module/Fluid\_Flow/fractured\_reservoir\_flow

# Fluid (Fracture)

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

## MODEL INPUT

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

## FLUID PROPERTIES

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

## Gas/Liquid

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

## Ideal Gas

For Ideal gas it uses the ideal gas law to describe the fluid. In this case, specify the thermodynamics properties. Select a Gas constant type — Specific gas constant  $R_s$  (the default) or Mean molar mass  $M_n$  (SI unit:  $J/(mol \cdot K)$ ). 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  $\chi_f$ =  $1/p_A$  with the absolute pressure  $p_A$  (Pa).



If Hydraulic conductivity is selected as the Permeability model (see the Fracture Material section), dynamic viscosity is not available. The hydraulic conductivity is defined using a combination of fluid and fracture material properties and replaces the need of defining the dynamic viscosity.

# Fracture Material

This node defines the porosity and material properties of the solid matrix of the Fracture parent node.

## MODEL INPUT

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

## BARRIER PROPERTIES

This section appears if the Thin conducting barrier option for the Fracture model is chosen in the parent Fracture feature.

Enter the values for the barrier thickness  $d_{\rm b}$  and permeability  $\kappa_{\rm b}$ .

Note that the **Thin Conductive barrier** option is only available for the Fracture feature within the Darcy's Law interface.

## FRACTURE MATERIAL PROPERTIES

If the Thin conducting barrier option for the Fracture model is chosen in the parent Fracture feature you can specify the Conductive layer position here. Choose between Both sides, Upside, and Downside. A sketch above shows the position of conductive layers and barrier within the fracture.

The Porosity  $\varepsilon_{p}$  of the fracture material is taken From material by default. 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  $\chi_p = 10^{-4}$  1/Pa.

Select a **Permeability model** to specify the capacity of the fracture material to transmit flow. Which options are available depends on the Flow model setting in the parent node.

- Select **Permeability** (default) to define the permeability of the fracture material.
- Select **Hydraulic conductivity** or define a combination of fluid permeability and dynamic viscosity. For Hydraulic conductivity K (SI unit: m/s) select Isotropic to define a scalar value or **Diagonal** or **Symmetric** to define a tensor value. The default is  $2.94 \cdot 10^{-4} \text{ m/s}.$
- Select Cubic law to define the permeability from the fracture thickness specified in the parent node and the roughness factor  $f_{\rm f}$ .

If the Non-Darcian Flow Model is selected in the parent Fracture feature enter a value for the Inertial resistance coefficient  $\beta$ .



- 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

# 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.

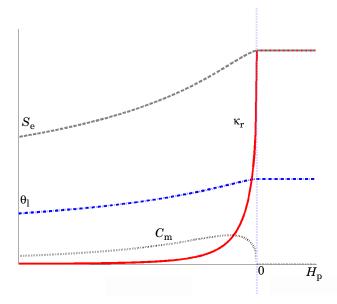


Figure 4-1: Fluid retention and permeability functions that vary with pressure head, as given by Van Genuchten formulas available in the Richards' Equation interface.

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):

$$\rho \left( \frac{C_{\rm m}}{\rho g} + S_{\rm e} S_{\rm p} \right) \frac{\partial p}{\partial t} + \nabla \cdot \rho \left( -\frac{\kappa_{\rm r} \kappa_{\rm s}}{\mu} (\nabla p + \rho g \nabla D) \right) = Q_{\rm m}$$
 (4-26)

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,  $\kappa_s$  gives the hydraulic permeability at saturation,  $\mu$  is the fluid dynamic viscosity,  $\kappa_r$  denotes the relative permeability,  $\rho$  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

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

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,  $\theta_l$ . This interstitial, pore or average linear velocity is  $\mathbf{u}_a = \mathbf{u}/\theta_1$ .

# 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  $\theta_l$ ,  $S_e$ ,  $C_m$ , and  $\kappa_r$  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,  $\theta_l$ , ranges from a small residual value  $\theta_r$  to the total porosity  $\varepsilon_p$ . Its value is given in a constitutive relation in the model commonly defined as:

$$\theta_1 = \theta_r + S_e(\theta_s - \theta_r) \tag{4-27}$$

The variable  $\theta_s$  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  $\theta_1$  versus pressure (or pressure head):

$$C_{\rm m} = \frac{\partial \theta_{\rm l}}{\partial H_{\rm p}}$$

The relative permeability,  $\kappa_r$ , 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  $\theta_l$ ,  $S_e$ ,  $C_m$ , and  $\kappa_r$ :

- 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  $\theta_s$  and residual  $\theta_r$  liquid volume fractions as well as constants  $\alpha$ , 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:

$$S_{c} = \begin{cases} \frac{1}{(1 + |\alpha H_{p}|^{n})^{m}} & H_{p} < 0 \\ 1 & H_{p} \ge 0 \end{cases}$$

For the liquid volume fraction Equation 4-27 is used. The relative permeability is defined as

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

which results in  $\kappa_r = 1$  at saturation ( $S_e = 1$ ). The specific moisture capacity is defined as:

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

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

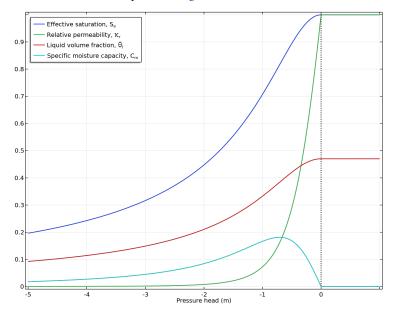


Figure 4-2: Van Genuchten retention functions for  $\alpha = 1 \text{ m}^{-1}$ , n = 2, and l = 0.5.

# **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

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

Again Equation 4-27 describes the liquid volume fraction. The relative permeability is defined as

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

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

$$C_{\rm m} = \begin{cases} \frac{-n}{H_p} (\theta_{\rm s} - \theta_{\rm r}) S_{\rm c} & H_p < -\frac{1}{\alpha} \\ 0 & -\frac{1}{\alpha} \le H_p \end{cases}$$

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

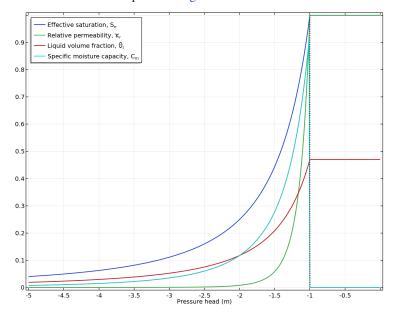


Figure 4-3: The Brooks and Corey retention functions for  $\alpha = 1 \text{ m}^{-1}$ , n = 2, and l = 0.5.

## 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  $\theta_l, S_e, C_m$ , and  $\kappa_r$  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. Clear 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/s<sup>2</sup>). 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

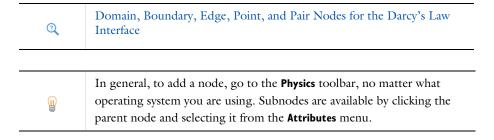
You can choose the order of the shape functions used for the pressure variable solved by the Richards' Equation interface. The default shape functions are Quadratic Lagrange.

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

• Theory for the Richards' Equation Interface • Domain, Boundary, Edge, Point, and Pair Nodes for the Richards' 2 **Equation Interface** • Physical Constants in the COMSOL Multiphysics Reference Manual • Variably Saturated Flow: Application Library path Subsurface\_Flow\_Module/Fluid\_Flow/variably\_saturated\_flow 1111 • 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.







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 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:

$$\mathbf{q}_{\mathrm{f}} = -\frac{\kappa_{\mathrm{f}}}{\mu} d_{\mathrm{f}} (\nabla_{\mathrm{T}} p + \rho \, g \, \nabla_{\mathrm{T}} D) \tag{4-28}$$

Here,  $\mathbf{q}_f$  is the volume flow rate per unit length in the fracture,  $\kappa_f$  is the fracture's permeability,  $\mu$  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,  $\rho$  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  $\mathbf{u}_f = \mathbf{q}_f/d_f$ .

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  $\kappa_f$ and fluid viscosity  $\mu$ . 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  $d_{\rm f}$  and the roughness factor  $f_{\rm f}$ 

$$\kappa_{\rm f} = \frac{d_{\rm f}^2}{12f_{\rm f}}$$

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.

$$d_{f} \frac{\partial}{\partial t} (\varepsilon_{f} \rho) + \nabla_{T} \cdot (\rho \mathbf{q}_{f}) = d_{f} Q_{m}$$
 (4-31)

where  $\varepsilon_f$  is the fracture porosity, and  $Q_m$  is the mass source term (SI unit: kg/(m<sup>3</sup>·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  $S_f$  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 (ff) interface ( ), found under the Porous Media and Subsurface Flow branch ( ) when adding a physics interface, is used to simulate flow along faults and fractures represented as boundaries. 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 — Fracture, 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 ff.

## PHYSICAL MODEL

Enter a **Reference pressure level**  $p_{ref}$  (SI 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 ( **a**) and select **Advanced Physics Options.** 

2

- 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

- Fracture
- Initial Values
- · Unsaturated Porous Medium
- Mass Source
- 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
- Precipitation

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.

# Fracture

The Fracture feature for the Fracture Flow interface uses the same settings as the Fracture boundary condition for Darcy's Law except that the fracture model is not available. With the Fracture Flow interface, only highly conductive fractures can be modeled.

As the Fracture boundary condition, the Fracture feature has two subfeatures: Fluid (Fracture) and Fracture Material.

# 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  $H_p$  (SI unit: m).
- Select Hydraulic head to enter a value or expression for H (SI unit: m).

# Theory for the Layered Darcy's Law Interface

The Theory for the Layered Darcy's Law interface is based on Darcy's Law which is described in Theory for the Darcy's Law Interface. Therefore, this section focuses on the 2D approximation for layered materials.

The Darcy's Law with continuity equation can be found in Section Theory for the Darcy's Law Interface, Equation 4-2. The Darcy velocity can be written as:

$$\mathbf{u} = -\frac{\kappa}{\mu} (\nabla p - \rho g \nabla D) \tag{4-32}$$

where  $\kappa$  is the permeability of porous material,  $\mu$  is the dynamic viscosity of fluid,  $\rho$  the fluid density, p is the fluid pressure, g is the gravitational constant, and D is the elevation.

# Gradient Handling

In thin structures, the tangential gradient and the normal gradient can be more appropriate to express the governing equations. The normal gradient is the projection of the gradient operator onto the normal vector,  $\mathbf{n}$ , of the boundary representing the thin structure. This is mathematically expressed for any scalar field p as:

$$\nabla_{\mathbf{n}}p = (\nabla p \cdot \mathbf{n})\mathbf{n} .$$

The tangential gradient removes the normal component from the gradient operation, so that only tangential components remain. This is mathematically expressed for any scalar field p as:

$$\nabla_{\mathbf{t}} p = \nabla p - (\nabla p \cdot \mathbf{n}) \mathbf{n} .$$

The gradient operator is then split into a tangential part and a normal part:

$$\nabla p = \nabla_{\mathbf{t}} p + \nabla_{\mathbf{n}} p . \tag{4-33}$$

Equation 4-33 is valid for flat layered shells. However, for curved shells, the gradient expression should account for the surface area and the scaling of each layer. The

gradient in the product geometry of a curved layered shell with variable thickness can be written as:

$$\nabla p = \left[ \left( \frac{\partial \mathbf{X}}{\partial \mathbf{X}_r} \right)^{-1} \right]^{\mathrm{T}} \cdot (\nabla_{\mathbf{t}} p + \nabla_{\mathbf{n}} p) .$$

In some applications, it is required to model variable thickness layers. This is achieved by scaling the constant thickness of the layer, d, using a thickness factor,  $l_{sc}$ , which can be a function of the surface coordinates. The deformation gradient in a scaled product geometry of a curved layered shell can be written as

$$\nabla p = \left[ \left( \frac{\partial \mathbf{X}}{\partial \mathbf{X}_{r}} \right)^{-1} \right]^{T} \cdot \left( \nabla_{\mathbf{t}} T + \frac{\nabla_{\mathbf{n}} p}{l_{sc}} \right)$$

It should be noted that when an extra dimension is used, the equations are written from the point of view of the extra dimension. In particular, the dtang() operator would correspond to  $\nabla_{\mathbf{n}}$  since it performs the derivation along the extra line.

Then, the gradient becomes

$$\nabla p = \left[ \left( \frac{\partial \mathbf{X}}{\partial \mathbf{X}_r} \right)^{-1} \right]^{\mathsf{T}} \cdot \left( \nabla_{t} p + \frac{\mathrm{dtang}(p, x_d)}{l_{sc}} \cdot \mathbf{n}^T \right)$$

where  $x_d$  is the extra dimension coordinate,  $\bf n$  is the positive normal direction, and

$$\frac{\partial \mathbf{X}}{\partial \mathbf{X}_{e}} = \mathbf{I} + \left(z + \frac{d}{2}(-1 + z_{\text{off}})\right)\nabla_{\mathbf{t}}\mathbf{n}$$

where

- $\mathbf{X}_{r}$  are the reference surface coordinates
- z is the extra-dimension thickness coordinate (varying between 0 and d)
- $z_{\text{off}}$  is the relative midplane offset
- d is the layered material thickness.

# Area Scale Factor

For a curved layered shell, the change in surface area of each layer should be accounted for while integrating the governing equations. The area scale factor for each layer of the layered material can be defined as

# Related information:

- Modeling Layered Materials in the Heat Transfer Module User's Guide
- Results Evaluation in Layered Shells in the Structural Mechanics User's Guide

2

- See Layered Material, Layered Material Slice, and Through Thickness in the COMSOL Multiphysics Reference Manual for details about the Layered Material dataset, and slice and through-thickness plots in layered materials.
- Using Extra Dimensions in the COMSOL Multiphysics Reference Manual.

# The Layered Darcy's Law Interface

The Layered Darcy's Law (Idl) interface ( ), found under the Porous Media and **Subsurface Flow** branch ( ) when adding a physics interface, is used to simulate flow within layered porous materials which are defined on boundaries within a 3D model domain. It is only available for 3D simulations and is only active on all boundaries where a layered material is defined.

> A layered material can be defined on the boundaries by adding one of the following nodes:

- Single Layer Material
- Layered Material Link, together with a Layered Material node
- Layered Material Stack, together with one or several Layered Material nodes
- Material, with the Layer thickness property specified

See Lavered Material, Lavered Material Link, Lavered Material Stack, Layered Material Link (Subnode), and Single Layer Materials in the COMSOL Multiphysics Reference Manual for details on the definition of lavered materials.

The physics interface uses a variant of Darcy's law and can be used for stationary and time-dependent analysis. Although the layered material is represented as a boundary in the model, the through-thickness variation of the pressure is accounted for. In addition, a single boundary may represent several layers with different properties varying through the thickness of the layered material. This uses the Extra Dimension tool which defines the equations on the product space between the boundary and the additional dimension for the thickness of the layered material.

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

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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 1d1.

#### SHELL PROPERTIES

Here you select specific layers in a layered material on which the physics interface should be active. By default, the **Use all layers** check box is selected. This means that all layers in all layered materials on the selected boundaries are used.

If you clear the Use all layers check box, you can select individual layers within a single layered material. This means that the physics interface is restricted to the boundaries on which a specific layered material is defined.



For a general description of layer selections, see The Shell Properties and Interface Selection Sections in the Structural Mechanics Module User's Guide.

# PHYSICS SYMBOLS

There are physics symbols available with some physics features to help you to graphically indicate boundary conditions, boundary normal orientation, loads, and other features. To display them select the **Enable Physics Symbols** check box under Physics Symbols in the Settings window. You can click the Select All button, which displays all symbols in that physics interface by selecting all **Show physics symbols** check boxes in the Settings windows for the physics features that include symbols. Similarly, the Clear All button clears all Show physics symbols check boxes in the individual physics features.



For a more detailed description of Physics Symbols, see Physics Symbols in the COMSOL Multiphysics Reference Manual.

#### PHYSICAL MODEL

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

## **GRAVITY EFFECTS**

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

Note that by default there are no gravity effects added to the Layered Darcy's Law interface. To activate the acceleration of gravity, add the **Gravity** feature node from the Physics toolbar or right-click Layered Darcy's Law to select it from the context menu.

## 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 Layered 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 selected. The smoothing can provide a better behaved flux value close to singularities.

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 details about the settings for boundary fluxes, see Computing Accurate Fluxes in the COMSOL Multiphysics Reference Manual.

• For more information on splitting complex-valued variables, see Splitting Complex-Valued Variables in the COMSOL Multiphysics Reference Manual.

## **DEPENDENT VARIABLES**

2

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

> · Boundary, Edge, and Point Nodes for the Layered Darcy's Law Interface

• Theory for the Layered Darcy's Law Interface

• Physical Constants in the COMSOL Multiphysics Reference Manual

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

The Layered Darcy's Law Interface has the following boundary, edge, and point nodes, which 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).

#### **BOUNDARY NODES**

- Fluid and Matrix Properties
- Gravity
- Initial Values
- · Storage Model

- Mass Source
- · Poroelastic Storage
- Richards' Equation Model

# **BOUNDARY INTERFACE NODES**

- Pressure, Interface
- Mass Flux, Interface
- Inlet, Interface
- Outlet, Interface
- Symmetry, Interface

- No Flow, Interface
- Flux Discontinuity, Interface
- Interior Wall, Interface
- Thin Barrier, Interface

## **EDGE NODES**

The following nodes (listed in alphabetical order) are available on edges. As most of the edge features are very similar to the boundary nodes of the Darcy's Law Interface, those links point to the feature descriptions there. Also take a look at Section Edge Features below.

- Continuity
- Flux Discontinuity
- Inlet
- Line Mass Source, Interface
- Mass Flux

- No Flow
- Outlet
- Pressure
- Symmetry

#### **POINT NODES**

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

• Line Mass Source

· Point Mass 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.

# Fluid and Matrix Properties

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

## SHELL PROPERTIES

These settings can only be edited if the Fluid and Matrix Properties node was added manually. For the default node, the same settings as in the Shell Properties section of the parent interface are applied.

If you clear the **Use all layers** check box, you can select individual layers within one layered material. If you have defined more than one layered material in the model, this means that you would have to add another boundary node to define the physics in the remaining material sections.



For a general description of layer selections, see The Shell Properties and Interface Selection Sections in the Structural Mechanics Module User's Guide.

# MODEL INPUT

This section has fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs appear here. The default model input is the temperature T and the absolute pressure  $p_A$ .

#### FLUID PROPERTIES

For Fluid material you can select Boundary material (the default) to use the material defined on the boundary, or another material from the list to use that material's properties for the fluid.

Specify the density and dynamic viscosity as described in the Fluid section of The Darcy's Law Interface.

#### MATRIX PROPERTIES

For the porous matrix material, select either Boundary material from the Porous material list (the default) to use the material defined for the porous domain, or select another material to use that material's properties.

The matrix properties are defined as in The Darcy's Law Interface, so take a look at the Matrix Properties section for details.

# Initial Values

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

## SHELL PROPERTIES

The Shell Properties settings can only be edited if the Initial Values node was added manually. For the default node, the same settings as in the Shell Properties section of the parent interface are applied.

If you clear the Use all layers check box, you can select individual layers within one layered material. If you need to specify different initial values for different layered materials or for different layers, you have to add one Initial Values node for each layered material or for each layer.



For a general description of layer selections, see The Shell Properties and Interface Selection Sections in the Structural Mechanics Module User's Guide.

#### 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 licensed, 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.

# Richards' Equation Model

The Richards' Equation Model node defines the storage and retention models in variably saturated porous media. See the Unsaturated Porous Medium described for The Richards' Equation Interface.

Note that for the Layered Darcy's Law interface, the Fluid Properties and the Matrix **Properties** are defined on the boundary instead of the domain.

## SHELL PROPERTIES

In the Shell Properties section you determine on which layer the Richard's Equation Model is active. If you clear the **Use all layers** check box, you can select individual layers within one layered material. To specify different settings for different layered materials or for different layers, you have to add one boundary node for each layered material or for each layer, respectively. See also the Shell Properties section of the parent interface for more information.



For a general description of layer selections, see The Shell Properties and Interface Selection Sections in the Structural Mechanics Module User's Guide.

# Storage Model

The **Storage Model** node adds Equation 4-4 (excluding any mass sources). Use it to define the fluid and porous media properties, including a storage term for the specific storage.

# SHELL PROPERTIES

The settings are the same as for the Shell Properties section of the Richards' Equation Model node.

# **FLUID PROPERTIES**

The settings are the same as for the Fluid and Matrix Properties node except a gas constant type is not required.

#### MATRIX PROPERTIES

The settings are the same as in the Matrix Properties section under Fluid and Matrix Properties.

## STORAGE MODEL

Select a Storage S (SI unit: 1/Pa) — Linearized storage (the default) or User defined.

- For User defined enter a value or expression for Storage S (SI unit: 1/Pa).
- For Linearized storage it uses the following linear equation to define the storage:

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

This is equivalent to the Reuss average of the fluid and solid compressibilities. Enter the value or expression for each of the following:

- Compressibility of fluid  $\chi_f({\rm SI~unit:~1/Pa}).$  The default uses values From material. For **User defined**, the default is  $4 \cdot 10^{-10}$  1/Pa.

**Effective compressibility of matrix**  $\chi_D$  (SI unit: 1/Pa). The default is  $1 \cdot 10^{-4}$  1/Pa).

# Poroelastic Storage

The Poroelastic Storage node adds Equation 4-1 and Equation 4-4 (excluding any mass sources). Use it to define the fluid and porous media properties, including a storage term to account for the Poroelasticity multiphysics coupling.

## SHELL PROPERTIES

The settings are the same as for the Shell Properties section of the Richards' Equation Model node.

#### FLUID PROPERTIES

The settings are the same as for the Storage Model node except a gas constant type is not required. There is also an option to define the fluid compressibility.

# Compressibility

Select the Compressibility of fluid  $\chi_f(SI \text{ unit: } 1/Pa)$ . The default uses values From material as defined by the Fluid material selected. For User defined the default is  $4.10^{-10}$  1/Pa.

## MATRIX PROPERTIES

The settings are the same as in the Matrix Properties section under Fluid and Matrix Properties.

The **Gravity** node adds the acceleration of gravity to the simulation model.

#### SHELL PROPERTIES

The settings are the same as for the Shell Properties section of the Richards' Equation Model node.

## 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  $9.8066 \text{ m/s}^2$ .

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.

# Mass Source

The Mass Source node adds a mass source  $Q_m$ , which appears on the right-hand side of the Darcy's Law equation:

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

#### SHELL PROPERTIES

The settings are the same as for the Shell Properties section of the Richards' Equation Model node.

## MASS SOURCE

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

# Boundary Interface Features

The Layered Darcy's Law interface has several boundary interface nodes and subnodes available. These nodes apply boundary conditions to the exterior interfaces of a layered shell or to the interfaces between its layers.

# Pressure, Interface

Use the **Pressure**, **Interface** node to specify the pressure on the exterior interfaces of a layered shell or on the interfaces between its layers.

In many cases the distribution of pressure is known, giving a Dirichlet condition p = 1 $p_0$  where  $p_0$  is a known pressure given as a number, a distribution, or an expression involving time, t, for example.

# INTERFACE SELECTION

Set the interfaces for which the pressure should be specified. These can be internal interfaces between layers or the top and bottom surfaces.

The available options in the Apply to list are Top interface, Bottom interface, Exterior interfaces, Interior interfaces, All interfaces, and Selected interfaces. With the last option you can select any set of interfaces for a given layered material, by clearing the check boxes corresponding to layer interfaces where the node should not be applied in the Selection table. The top and bottom interfaces refer respectively to the upside and downside of the boundary, defined from the orientation of the normal vector. You can visualize the selected interfaces by clicking the Layer Cross Section Preview () and Layer 3D Preview ( ) buttons.



For a general description of layer and interface selections, see Layer and Interface Selection Tools in the Heat Transfer Module User's Guide.

#### PRESSURE

Enter a value or expression for the **Pressure**  $p_0(SI \text{ unit: Pa})$ .

#### CONSTRAINT SETTINGS

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

2

For detailed information about the Constraint settings menu see section Constraint Settings in the COMSOL Multiphysics Reference Manual.

# Mass Flux, Interface

Use the Mass Flux, Interface node to add a mass flux on the exterior interfaces of a layered shell.

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 specified inward (or outward) Darcy flux.

## INTERFACE SELECTION

Set the interfaces for which the mass flux should be specified. Note that it can only be applied to exterior interfaces of the layered shell.

The available options in the Apply to list are Top interface, Bottom interface, Exterior interfaces (which is the default setting) and Selected interfaces. With the last option you can select a set of interfaces and the layered material for which the boundary condition should be active. Note that the check boxes for internal interfaces between layers are deactivated for this node.

The top and bottom interfaces refer respectively to the upside and downside of the boundary, defined from the orientation of the normal vector. You can visualize the selected interfaces by clicking the Layer Cross Section Preview ( ) and Layer 3D **Preview** ( ) buttons.



For a general description of layer and interface selections, see Layer and Interface Selection Tools in the Heat Transfer Module User's Guide.

#### CONSTRAINT SETTINGS

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

2

For detailed information about the Constraint settings menu see section Constraint Settings in the COMSOL Multiphysics Reference Manual.

## MASS FLUX, INTERFACE

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:  $kg/(m^2 \cdot s)$ ).

# Inlet, Interface

The Inlet, Interface node adds an inflow condition to the exterior interfaces of a layered shell.

#### INTERFACE SELECTION

Set the interfaces for which the inflow should be specified. Note that the **Inlet, Interface** node can only be applied to exterior interfaces of the layered shell. The settings are the same as for the Interface Selection section of the Mass Flux, Interface node.

# **BOUNDARY CONDITION**

The available Boundary Condition options for an inlet are Velocity, Pressure, and Mass flow. 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

Enter a value or expression for the **Normal inflow velocity**  $U_0$  (SI unit: m/s). It is specified as  $\mathbf{u} = -\mathbf{n}U_0$ , where  $\mathbf{n}$  is the face normal and  $U_0$  is the normal inflow speed. A positive value of  $U_0$  represents an inflow velocity. A negative value represents an outflow velocity.

## PRESSURE

Enter a value or expression for the inlet **Pressure**  $p_0$  (SI unit: Pa).

#### MASS FLOW

If you select Mass flow as the inlet condition, you have to specify the Mass flow type, either as total Mass flow rate  $M_0$  (SI unit: kg/s), or the Pointwise mass flux  $N_0$  (SI unit:  $kg/(m^2 \cdot s)$ ).

With Mass flow rate boundary interface condition, positive values correspond to flow into the shell:

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

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

For the Pointwise mass flux boundary interface condition, positive values correspond to flow into the shell:

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

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 ( **a**) and select **Advanced** Physics Options in the Show More Options dialog box.



For detailed information about the Constraint settings menu see section Constraint Settings in the COMSOL Multiphysics Reference Manual.

# Outlet, Interface

The **Outlet**, **Interface** node adds an outflow condition to the exterior interfaces of a layered shell.

## INTERFACE SELECTION

Set the interfaces for which the outflow should be specified. Note that the **Outlet**, Interface node can only be applied to exterior interfaces of the layered shell. The settings are the same as for the Interface Selection section of the Mass Flux, Interface node.

#### **BOUNDARY CONDITION**

The available **Boundary Condition** options for an outlet are **Velocity** 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

Enter a value or expression for the **Normal outflow velocity**  $U_0$  (SI unit: m/s). It is specified as  $\mathbf{u} = \mathbf{n}U_0$ , so a positive value of  $U_0$  represents an outflow velocity whereas a negative value represents an inflow velocity.

#### PRESSURE

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

## CONSTRAINT SETTINGS

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



For detailed information about the Constraint settings menu see section Constraint Settings in the COMSOL Multiphysics Reference Manual.

# Symmetry, Interface

The Symmetry, Interface node adds a symmetry boundary condition to the external boundaries of a layered shell. The following condition implements the symmetry condition on an axis or a flow divide:

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

## INTERFACE SELECTION

Set the interfaces for which the symmetry condition should be specified. Note that it can only be applied to exterior interfaces of the layered shell.

The available options in the Apply to list are Top interface, Bottom interface, Exterior interfaces (which is the default setting), and Selected interfaces. With the last option you can select a set of interfaces and the layered material for which the boundary condition should be active. Note that the check boxes for internal interfaces between layers are deactivated for the symmetry, interface node.

The top and bottom interfaces refer respectively to the upside and downside of the boundary, defined from the orientation of the normal vector. You can visualize the selected interfaces by clicking the Layer Cross Section Preview ( ) and Layer 3D **Preview** ( ) buttons.

2

For a general description of layer and interface selections, see Layer and Interface Selection Tools in the Heat Transfer Module User's Guide.

# No Flow, Interface

The **No Flow, Interface** states that there is no flow across impermeable external boundaries of a layered shell. The mathematical formulation is:

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

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

#### INTERFACE SELECTION

Set the interfaces for which the no flow condition should be specified. Note that this node can only be applied to exterior interfaces of the layered shell. The settings are the same as for the Interface Selection section of the Mass Flux, Interface node.

# Flux Discontinuity, Interface

Use the Flux Discontinuity, Interface node to specify a mass flux discontinuity through an interior interface of a layered shell. The condition is represented by the following equation:

$$-\mathbf{n} \cdot \rho(\mathbf{u}_1 - \mathbf{u}_2) = N_0$$

In this equation, **n** is the vector normal (perpendicular) to the interior layer interface,  $\rho$  is the fluid density,  $\mathbf{u}_1$  and  $\mathbf{u}_2$  are the Darcy velocities in the adjacent domains, and  $N_0$  is a specified value or expression for the flux discontinuity.

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 layer interface.

# INTERFACE SELECTION

Set the interface for which the flux discontinuity should be specified. Note that this node can only be applied to interior interfaces of a layered shell.

The available options in the **Apply to** list are **Interior interfaces**, which is the default setting, and Selected interfaces. With the last option you can select a set of interfaces and the layered material for which the boundary interface condition should be active. Note that the check boxes for exterior interfaces of the layered material are deactivated for this node.

You can visualize the selected interfaces by clicking the Layer Cross Section Preview (**a**) and **Layer 3D Preview** (**a**) buttons.



For a general description of layer and interface selections, see Layer and Interface Selection Tools in the Heat Transfer Module User's Guide.

## FLUX DISCONTINUITY, INTERFACE

Enter a value or expression for the **Inward mass flux**  $N_0$  (SI unit: kg/(m<sup>2</sup>·s)). A positive value of  $N_0$  represents a mass flux discontinuity in the opposite direction to the normal vector of the interior boundary.

# Interior Wall, Interface

The Interior Wall, Interface condition can only be applied on interior interfaces of a layered shell. It is similar to the No Flux, Interface condition, except that it applies on interior interfaces and therefore on both sides of the interfaces. It allows discontinuities of velocity and pressure across the layer interface.

# INTERFACE SELECTION

Set the interface for which the Interior Wall, Interface condition should be specified. Note that this node can only be applied to interior interfaces of a layered shell.

The available options in the Apply to list are Interior interfaces, which is the default setting, and Selected interfaces. With the last option you can select a set of interfaces and the layered material for which the boundary interface condition should be active. Note that the check boxes for exterior interfaces of the layered material are deactivated for this node.

You can visualize the selected interfaces by clicking the Layer Cross Section Preview (**a**) and **Layer 3D Preview** (**a**) buttons.

2

For a general description of layer and interface selections, see Layer and Interface Selection Tools in the Heat Transfer Module User's Guide.

# Thin Barrier, Interface

The **Thin Barrier**, **Interface** condition models interior permeable interfaces like membranes, permeable walls, geotextiles, or perforated plates as thin permeable barriers. It can only be applied on interior interfaces of layered shells.

At the thin barrier interface, a discontinuity in the velocity field is modeled using the following equations:

$$-\mathbf{n}_{u} \cdot (\rho \mathbf{u})_{u} = \frac{\rho(p_{d} - p_{u}) \kappa_{b}}{\mu} \frac{\kappa_{b}}{d_{b}}$$

$$-\mathbf{n}_d \cdot (\rho \mathbf{u})_d = \frac{\rho(p_u - p_d)}{\mu} \frac{\kappa_b}{d_b}$$

where **n** is the vector normal to the interface, **u** the Darcy velocity,  $\rho$  the density and p the pressure. Subscript d denotes the downside of the interface, and u denotes the upside of the interface.  $\kappa_b$  is the permeability of the thin barrier material,  $d_b$  the barrier thickness.

# INTERFACE SELECTION

Set the interface for which the Thin Barrier, Interface node should be specified. Note that it can only be applied to interior interfaces of layered shells.

The settings are the same as for the Interface Selection section of the Interior Wall, Interface node.

#### 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 interface normal and of the velocity.

#### WALL

Enter a value or expression for the **Permeability**  $\kappa_b$  (SI unit: m<sup>2</sup>). The default Permeability  $\kappa_h$  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.

Enter a value or expression for the **Thickness**  $d_b$  (SI unit: m, the default is 0.1 m).

# Edge Features

Most of the edge feature nodes available with the Layered Darcy's Law Interface are very similar to the corresponding Boundary Interface Features nodes and are therefore not further described here. Instead of the Interface selection section the edge feature nodes have a **Shell Properties** section like the boundary nodes. The settings are the same as for example the Shell Properties section of the Richards' Equation Model node.

However, there are two special edge feature nodes which have no corresponding boundary interface node and are described below.

# Line Mass Source, Interface

The Line Mass Source, Interface node adds mass flow originating from a tube of infinitely small radius to edges of layer interfaces of layered shells.

#### INTERFACE SELECTION

Set the interfaces on whose edges the Line Mass Source, Interface condition should be applied. These can be internal interfaces between layers or the top and bottom surfaces.

The available options in the **Apply to** list are **Top interface** (the default setting), **Bottom** interface, Exterior interfaces, Interior interfaces, All interfaces, and Selected interfaces. With the last option you can select any set of interfaces for a given layered material, by clearing the check boxes corresponding to layer interfaces where the node should not be applied in the **Selection** table. The top and bottom interfaces refer respectively to the upside and downside of the boundary, defined from the orientation of the normal

vector. You can visualize the selected interfaces by clicking the Layer Cross Section **Preview** ( ) and Layer 3D Preview ( ) buttons.

2

For a general description of layer and interface selections, see Layer and Interface Selection Tools in the Heat Transfer Module User's Guide.

#### LINE MASS SOURCE. INTERFACE

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.



For more information see Mass Sources for Fluid Flow in the COMSOL Multiphysics Reference Manual.

# Continuity

Use this node to specify the side-by-side continuity conditions on the pressure field at an edge between two layered materials. By default, the pressure is discontinuous at the interface between two layered materials.

The continuity constraint is added on the common edge in the through-thickness direction.

#### LAYER SELECTION

Select **Source** and **Destination** layered materials from the drop-down lists. This makes the node applicable on the edges adjacent to both selected layered materials. An Offset can be specified on the destination side which decides the actual connection area between the two layered materials.

You can swap the source and destination by clicking **Swap Source and Destination** ( 1 ).

Click the **Layer Cross Section Preview** button to visualize the settings.

#### CONSTRAINT SETTINGS

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

# Point Features

The Layered Darcy's Law Interface has the following special point feature nodes:

# Line Mass Source

The Line Mass Source node adds mass flow originating from a tube of infinitely small radius. In case of a point feature, the tube lies along the virtual layer edge perpendicular to the layer surface.

#### SHELL PROPERTIES

In the **Shell Properties** section you determine on which layer edge the Line Mass Source is defined. You can select individual layers within one layered material. To specify different settings for different layered materials or for different layers within one layered material, you have to add one boundary node for each layered material or for each layer, respectively. You can visualize the selected layers by clicking the Layer Cross **Section Preview** (**()** and **Layer 3D Preview** (**()** buttons.

# 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.



For more information see Mass Sources for Fluid Flow in the COMSOL Multiphysics Reference Manual.

# Point Mass Source

The **Point Mass Source** node models mass flow originating from an infinitely small sphere centered around a point which lies on a layer interface of a layered material.

# INTERFACE SELECTION

Set the interfaces on whose points the **Point Mass Source** condition should be applied. These can be internal interfaces between layers or the top and bottom surfaces.

The available options in the Apply to list are Top interface (the default setting), Bottom interface, Exterior interfaces, Interior interfaces, All interfaces, and Selected interfaces. With the last option you can select any set of interfaces for a given layered material, by clearing the check boxes corresponding to layer interfaces where the node should not be applied in the **Selection** table. The top and bottom interfaces refer respectively to the upside and downside of the boundary, defined from the orientation of the normal vector. You can visualize the selected interfaces by clicking the Layer Cross Section **Preview** () and **Layer 3D Preview** () buttons.



For a general description of layer and interface selections, see Layer and Interface Selection Tools in the Heat Transfer Module User's Guide.

# 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.

# 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:

$$\frac{\partial}{\partial t}(\varepsilon_{\rm p}\rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m} \tag{4-34}$$

$$\begin{split} &\frac{\rho}{\varepsilon_{\mathrm{p}}} \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon_{\mathrm{p}}} \right) = \\ &- \nabla p + \nabla \cdot \left[ \frac{1}{\varepsilon_{\mathrm{p}}} \left\{ \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} \right] - \left( \kappa^{-1} \mu + \frac{Q_{\mathrm{m}}}{\varepsilon_{\mathrm{p}}^{2}} \right) \mathbf{u} + \mathbf{F} \end{split}$$

In these equations:

- $\mu$  (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- **u** (SI unit: m/s) is the velocity vector
- $\rho$  (SI unit: kg/m<sup>3</sup>) is the density of the fluid
- p (SI unit: Pa) is the pressure
- $\varepsilon_{\rm p}$  is the porosity
- $\kappa$  (SI unit: m<sup>2</sup>) is the permeability of the porous medium, and
- $Q_{\rm m}$  (SI unit: kg/(m<sup>3</sup>·s)) is a mass source or sink

Influence of gravity and other volume forces can be accounted for via the force term  $\mathbf{F}$  (SI unit:  $kg/(m^2 \cdot s^2)$ ).

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 4-35 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 4-35; see References for the Darcy's Law Interface for details.

In case of a flow with variable density, Equation 4-34 and Equation 4-35 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

$$\frac{\partial}{\partial t}(\varepsilon_{\rm p}\rho) + \mathbf{u} \cdot \nabla \rho = 0$$

and the continuity equation (Equation 4-34) reduces to

$$\rho \nabla \cdot \mathbf{u} = Q_{m}$$

# References for the Brinkman Equations Interface

- 1. D. Nield and A. Bejan, Convection in Porous Media, 3rd ed., Springer, 2006.
- 2. M. Le Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," J. Fluid Mech., vol. 550, pp. 149-173, 2006.

# The Brinkman Equations Interface

The Brinkman Equations (br) interface ( ), found under the Porous Media and **Subsurface Flow** branch ( ) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. The physics interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. To simplify the equations, select the Stokes-Brinkman flow feature to reduce the dependence on inertial effects when the Reynolds number is significantly less than 1. The physics interface can be used for stationary and time-dependent analyses.

The main node is the Porous Medium feature, which adds the Brinkman equations and provides interfaces for defining the fluid material and the porous matrix.

When this physics interface is added, the following default nodes are also added in the Model Builder — Porous Medium, Wall (the default boundary type, using No slip as the default boundary condition), and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Brinkman Equations** to select physics features from the context menu.

The boundary conditions are essentially the same as for the Laminar Flow interface. Differences exist for the following boundary types: Outlet, Symmetry, Open Boundary, and Boundary Stress where the viscous part of the stress is divided by the porosity to appear as

$$\frac{1}{\varepsilon_{p}} \left\{ \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right\}$$

In the COMSOL Multiphysics Reference Manual see Table 2-4 for links to common sections such as Discretization, Consistent Stabilization, Inconsistent Stabilization, and **Advanced Settings**, all accessed by clicking the **Show** button ( **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  $u_0$  in the azimuthal direction. While  $u_{\varphi}$  can be nonzero, there can be no gradients in the  $\varphi$  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 and Porous slip (default). The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in the 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  $T_{\rm ref}$  (SI unit: K). The default value is 293.15[K].

Reference Position

If Include gravity is selected, a Reference position  $r_{\mathrm{ref}}(\mathrm{SI~unit:m})$  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). If turbulent flow is activated, you can set the Turbulence model either to one of the algebraic turbulence models, Algebraic yPlus (the default) or **L-VEL**, or to one of the following two-equation turbulence models:  $k-\varepsilon$ , Low Reynolds Number k- $\epsilon$ . The **Wall treatment** is set to **Automatic** (default) or **Low Re** while **Wall functions** is the only option for k- $\epsilon$ . 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 ( **a** ) 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
- Theory for the Brinkman Equations Interface
- 2
- Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Steppingin the COMSOL Multiphysics Reference Manual
- Numerical Stability Stabilization Techniques for Fluid Flow
- Nitsche Constraints

Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface

The Brinkman Equations Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the Physics ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



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

These nodes are described in this section:

- Porous Medium
- Initial Values
- Mass Source

- Volume Force
- Fluid Properties

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

- Flow Continuity
- Inlet
- Line Mass Source
- · Boundary Stress
- Outlet
- Open Boundary

- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Wall



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

# Porous Medium

The **Porous Medium** node adds the Brinkman equations: Equation 4-34 and Equation 4-35 (excluding any mass sources). It has two default subfeatures — the Fluid subfeature where the fluid density  $\rho(SI \text{ unit: kg/m}^3)$  and dynamic viscosity  $\mu(SI \text{ subfeature})$ unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability κ (SI unit:  $m^2$ ) and porosity  $\varepsilon_p$  (dimensionless) are specified.

# COORDINATE SYSTEM SELECTION

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

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

#### FLOW MODEL

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

- Darcian flow (default) defines a linear relationship characteristic for low Reynolds number laminar flows.
- Non-Darcian flow defines a nonlinear relationship due to inertial or turbulence effects.

# POROUS MEDIUM TURBULENCE MODEL

If in the parent feature node a turbulence model other than Algebraic yPlus or L-VEL is selected, define a model which complements the basic turbulence model and accounts for the influence of the porous matrix on turbulent flow in porous media.

- For Default and Nakayama-Kuwahara specify the Coefficient of subgrid turbulence generation by porous matrix  $C_{\text{stpm}}$  which by default is set to 0.212.
- For Pedras-de Lemos, specify the Choice of the Pedras-de Lemos model coefficient. When User defined is chosen, specify the Coefficient of subgrid turbulence generation by porous matrix  $C_{\text{stpm}}$  with default value 0.212. Choosing Original results in  $C_{\text{stpm}} = 0.28 \cdot \sqrt{\varepsilon_p}$ , while choosing **Recalibrated** results in  $C_{\text{stpm}} = 0.18$ .

## DISTANCE EQUATION

This section is available for the turbulence models Algebraic yPlus or L-VEL. Select how the Reference length scale  $l_{ref}$  (SI unit: m) is defined — Automatic (default) or Manual:

- For Automatic the wall distance is automatically evaluated to one tenth of the shortest side of the geometry bounding box. This is usually quite accurate but it can sometimes give a too high value if the geometry consists of several slim entities. In such cases, define the reference length scale manually.
- For Manual it defines a different value or expression for the length scale. The default is 1 m.

 $l_{
m ref}$  controls the result of the distance equation. Objects that are much smaller than  $l_{
m ref}$ are effectively be diminished while the distance to objects much larger than  $l_{\mathrm{ref}}$  are accurately represented.

# 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**  $\rho$  and the **Dynamic viscosity**  $\mu$  (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 or **Symmetric** to define a tensor value.

For Kozeny-Carman, enter the mean Particle diameter  $d_{
m p}$  (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  $\kappa$  is then calculated using Equation 2-4.



- About Darcian and Non-Darcian Flow
- · Permeability Models

# Mass Source

The Mass Source node adds a mass source (or mass sink)  $Q_{
m m}$  to the right-hand side of the continuity equation: Equation 4-34. This term accounts for mass deposit and/or mass creation in porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

$$\frac{\partial}{\partial t}(\varepsilon_{p}\rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{m}$$
 (4-36)

#### 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/(m<sup>3</sup>·s)). The default is  $0 \text{ kg/(m}^3 \cdot \text{s})$ .

# Volume Force

Use the **Volume Force** node to specify the force  $\mathbf{F}$  on the right-hand side of Equation 4-35. It then acts on each fluid element in the specified domains.

$$\begin{split} &\frac{\rho}{\varepsilon_{p}} \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon_{p}} \right) = \\ &- \nabla p + \nabla \cdot \left[ \frac{1}{\varepsilon_{p}} \left\{ \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} \right] - \left( \kappa^{-1} \mu + \frac{Q_{m}}{\varepsilon_{p}^{2}} \right) \mathbf{u} + \mathbf{F} \end{split}$$

$$(4-37)$$

#### **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 ( **if** ) and entering the desired value in the input field.

#### FLUID PROPERTIES

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible.

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

# 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, Brinkman Interface

The Free and Porous Media Flow, Brinkman Interface uses the Navier-Stokes equations to describe the flow in open regions, and the Brinkman equations to describe the flow in porous regions.

The same fields, **u** and p, are solved for in both the free flow domains and in the porous domains. This means that the pressure in the free fluid and the pressure in the pores is continuous over the interface between a free flow domain and a porous domain. It also means that continuity is enforced between the fluid velocity in the free flow and the Darcy velocity in the porous domain. This treatment is one of several possible models for the physics at the interface. Examples of other models can be found in Ref. 1.

The continuity in  $\mathbf{u}$  and p implies a stress discontinuity at the interface between a free-flow domain and a porous domain. The difference corresponds to the stress absorbed by the rigid porous matrix, which is a consequence implicit in the formulations of the Navier-Stokes and Brinkman equations.

Reference for the Free and Porous Media Flow, Brinkman Interface

1. M.L. Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," J. Fluid Mech., vol. 550, pp. 149-173, 2006.

# The Free and Porous Media Flow, Brinkman Interface

The Free and Porous Media Flow, Brinkman (fp) interface ( ) is found under the Porous Media and Subsurface Flow branch ( No when adding a physics interface. It is used to compute fluid velocity and pressure fields of single-phase flow where free flow is connected to porous media. The Free and Porous Media Flow, Brinkman interface is used over at least two different domains: a free channel and a porous medium. The physics interface is well suited for transitions between slow flow in porous media, governed by the Brinkman equations, and fast flow in channels described by the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. The physics interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the Model Builder — Fluid Properties, Wall, and Initial Values. Then, from the Physics toolbar, add a **Porous Medium** node to be used on the domain selection corresponding to the porous media, or add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click Free and Porous Media Flow, **Brinkman** to select physics features from the context menu.

#### SETTINGS

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

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

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

#### PHYSICAL MODEL

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Navier-Stokes and Brinkman equations to model constant density flow. If required, select

Weakly compressible flow from the Compressibility list, to account for small variations in the density, which are only dependent on the temperature (nonisothermal flow) or Compressible flow (Ma<0.3) for fully compressible flow. However, for the flow modeled with this physics interface, the Mach number must be below 0.3.

Swirl Flow

For 2D axisymmetric components, select the **Swirl flow** check box to include the swirl velocity component, that is the velocity component  $u_0$  in the azimuthal direction. While  $u_{\varphi}$  can be nonzero, there can be no gradients in the  $\varphi$  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 and Porous slip (default). The latter option provides a unified treatment when the porous matrix is fully resolved as well as when it is under resolved ensuring a smooth transition between regions with different resolutions; see No Slip under Wall in the 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

Enter a Reference temperature  $T_{ref}$  (SI unit: K). The default value is 293.15[K].

Reference Position

If **Include gravity** is selected, a **Reference position**  $r_{ref}$  (SI unit: m) can be specified which is then used for the calculation of the hydrostatic pressure.

#### TURBULENCE

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS** (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, Brinkman Interface
- Theory for the Free and Porous Media Flow, Brinkman Interface

Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow, Brinkman Interface

The Free and Porous Media Flow, Brinkman Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the Physics ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



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

- Fluid Properties
- Gravity
- Initial Values

- Porous Medium
- · Mass Source
- Volume Force
- Wall

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

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

- No Viscous Stress
- Flow Continuity
- Inlet
- Line Mass Source
- Outlet

- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry



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

# Fluid Properties

Use the Fluid Properties node to define the fluid material, density, and dynamic viscosity.

#### **FLUID PROPERTIES**

The default Fluid material uses the Domain material (the material defined for the domain). Select another material as needed.

The default **Density**  $\rho$  (SI unit: kg/m<sup>3</sup>) uses values **From material** based on the **Fluid** material selection. For User defined enter another value or expression. The default is  $0 \text{ kg/m}^3$ .

The Dynamic viscosity  $\mu$  (SI unit: Pa·s) uses values From material based on the Fluid material selection. For User defined enter another value or expression. The default is O 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 p(SI unit: kg/m<sup>3</sup>) and dynamic viscosity  $\mu$  (SI unit: Pa·s) are defined and the Porous Matrix subfeature where the permeability  $\kappa$  (SI unit: m<sup>2</sup>) 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 characteristic for low Reynolds number laminar flows.
- Non-Darcian flow defines a nonlinear relationship due to inertial or turbulence effects.

## POROUS MEDIUM TURBULENCE MODEL

Defines a model which complements the basic turbulence model and accounts for the influence of the porous matrix on turbulent flow in Porous Media.

- Default and Nakayama-Kuwahara specify Coefficient of subgrid turbulence generation by porous matrix  $C_{\text{stpm}}$  which by default is set to 0.212.
- Pedras-de Lemos asks to specify Choice of the Pedras-de Lemos model coefficient. When User defined is chosen, specify Coefficient of subgrid turbulence generation by porous matrix C<sub>stom</sub> with default value 0.212. Choosing Original results in  $C_{stpm} = 0.28 \cdot \sqrt{\varepsilon_p}$ , while choosing **Recalibrated** results in  $C_{stpm} = 0.18$ .

### Fluid

This node defines the material properties of the fluid of the Porous Medium parent node.

#### MODEL INPUT

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

#### **FLUID PROPERTIES**

Specify the **Density**  $\rho$  and the **Dynamic viscosity**  $\mu$  (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 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 or **Symmetric** to define a tensor value.

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  $\kappa$  is then calculated using Equation 2-4.



- · About Darcian and Non-Darcian Flow
- · Permeability Models

# Mass Source

Enter a value or expression for an optional mass source (or sink) Source term  $Q_{\mathrm{m}}$  (SI unit: kg/(m<sup>3</sup>·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  $-g_{const}\mathbf{e}_{\mathbf{v}}$  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 Slip<sup>1</sup>

· 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 ( **a**) and selecting **Advanced Physics Options.** 



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

# Theory for the Free and Porous Media Flow, Darcy Interface

The Free and Porous Media Flow, Darcy interface uses the Navier-Stokes equations to describe the flow in the free-flow region, implemented by the coupled Laminar Flow interface, and Darcy's law, implemented by the coupled Darcy's Law interface, to describe the flow in the porous region.

In the free-flow region, the velocity u and pressure p are solved for, whereas in the porous region only the pressure p is solved for, and the velocity is calculated from the pressure by Darcy's law.

The coupling between the free and porous medium flow, implemented by the Free and Porous Media Flow Coupling, ensures conservation of mass across the free-porous interface, which is enforced by the condition

$$\mathbf{n} \cdot (\rho_{\text{ns}} \mathbf{u}_{\text{ns}}) = \mathbf{n} \cdot (\rho_{\text{d}} \mathbf{u}_{\text{d}}) \tag{4-38}$$

Here  $\rho_{ns}$  and  $\mathbf{u}_{ns}$  are the density and velocity on the free-flow side of the interface,  $\rho_d$ and  $\mathbf{u}_{d}$  the density and velocity on the porous side, and  $\mathbf{n}$  is a vector normal to the interface. In addition the coupling enforces the balance of the normal forces by:

$$p_{\rm ns} - \mathbf{n} \cdot \mathbf{Kn} = p_{\rm d} \tag{4-39}$$

where  $p_{ns}$  and  $p_{d}$  are the pressure on the free-flow side and porous side of the interface, respectively, and **K** is the viscous stress tensor (defined only on the free-flow side).

For the coupling condition for the tangential velocity component, there are several options. One of the most widely used conditions is the Beavers-Joseph interface condition (Ref. 1):

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{u}_{\text{ns}} - \mathbf{u}_{\text{d}}) = \frac{\sqrt{\text{tr}(\kappa)/n}}{\mu_{\text{ns}}\alpha_{BJ}}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n}$$
(4-40)

where  $a_{BJ}$  is the Beavers and Joseph parameter,  $\kappa$  is the permeability tensor of the porous medium (defined on the porous side of the interface),  $\mu_{ns}$  is the fluid's dynamic viscosity on the free-flow side of the interface, and n is the number of space dimensions.

When the velocity in the porous domain is much smaller than the velocity in the free flow, one can use a modification of the Beavers–Joseph condition which is given by the **Beavers–Joseph–Saffman** interface condition (Ref. 2):

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{u}_{\text{ns}} = \frac{\sqrt{\text{tr}(\kappa)/n}}{\mu_{\text{ns}}\alpha_{BJ}}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n}$$
(4-41)

For cases when the permeability tensor is not isotropic, the **Use projected permeability** option allows to take into account only the permeability in the direction of the tangential velocity component. This is accomplished by replacing the  $\sqrt{\text{tr}(\kappa)/n}$  term on the rights hand side of Equation 4-40 and Equation 4-41 by:

$$\sqrt{\mathbf{t} \cdot \kappa \mathbf{t}}$$
 (4-42)

with  $\mathbf{t}$  a unit vector tangent to the interface for 2D and 2D-axisymmetric cases, and for 3D cases by:

$$\sqrt{\mathbf{v} \cdot \kappa \mathbf{v}}$$
 (4-43)

with **v** given by:

$$\mathbf{v} = \frac{(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \mathbf{K} \mathbf{n}}{\|(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \mathbf{K} \mathbf{n}\|}$$
(4-44)

If one considers the limit of the Beavers–Joseph condition for large values of the Beavers and Joseph parameter  $a_{BJ}$ , one obtains the Continuous tangential velocity condition:

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{u}_{\text{ns}} - \mathbf{u}_{\text{d}}) = 0 \tag{4-45}$$

The same limit for the Beavers–Joseph–Saffman condition results in the No slip condition:

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{u}_{\mathbf{n}s} = 0 \tag{4-46}$$

The Viscous slip condition allows for a more general coupling condition. This interface condition is given by:

$$(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{u}_{ns} - \mathbf{u}_{b}) = \frac{L_{s}}{\mu_{ns}}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{K}\mathbf{n}$$
(4-47)

Here  $L_s$  is a slip length, and  $\mathbf{u}_{\mathrm{b}}$  a user-defined interfacial velocity.

Please find related information in the CFD Module User's Guide:

- The Darcy's Law Interface
- The Thin-Film and Porous Media Flow Interface
- The Laminar Flow Interface
- Theory for the Single-Phase Flow Interfaces

# References

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- 1. G.S. Beavers and D.D. Joseph, "Boundary Conditions at a Naturally Permeable Wall," J. Fluid Mech., vol. 30, 1967.
- 2. P.G. Saffman, "On the Boundary Condition at the Surface of a Porous Medium," Stud. Appl. Maths, vol. 50, 1971.

# The Free and Porous Media Flow, Darcy Interface

The Free and Porous Media Flow, Darcy interface ( ) combines the Darcy's Law and **Laminar Flow** interfaces to compute fluid velocity and pressure fields where free flow is connected to porous media. The physics interface is suited for situations when both the free flow and the flow in the porous media are laminar.

When a predefined Free and Porous Media Flow, Darcy interface is added from the Porous Media and Subsurface Flow branch ( ) of the Model Wizard or Add Physics window, the Darcy's Law and Laminar Flow interfaces are added to the Model Builder. In addition, the Multiphysics node is added, which automatically includes the Free and Porous Media Flow Coupling multiphysics coupling.

On the Constituent Physics Interfaces

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows in media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

The **Laminar Flow** interface is used to compute the velocity and pressure for a fluid flow in the laminar flow regime. A flow will remain laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence.

#### SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example Free and Porous Media Flow, Darcy, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

Free and Porous Media Flow Coupling (Multiphysics Coupling)

The Free and Porous Media Flow Coupling multiphysics coupling node ( ) bidirectionally links the Laminar Flow and Darcy's Law interfaces.

#### SETTINGS

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

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

The default **Name** (for the first multiphysics coupling feature in the model) is nsd1.

#### DOMAIN SELECTION

When nodes are added from the context menu, you can select Manual (the default) from the **Selection** list to choose specific domains to define the multiphase flow coupling, or select All domains as needed.

When the Free and Porous Media Flow Coupling is added as an effect of adding a Free and Porous Media Flow, Darcy multiphysics interface, the selection is the intersection of the boundaries of the participating physics interfaces.

Only boundaries that are active in the participating physics interfaces (which are chosen from the **Coupled Interfaces** selection list) can be selected.

#### COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Free flow** and **Porous media flow** lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the Model Wizard or Add Physics window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Free and Porous Media Flow Coupling node from a physics interface. If the physics interface is removed from the Model Builder, for example Darcy's Law is deleted, then the Porous media flow list defaults to **None** as there is nothing to couple to.

#### **COUPLING SETTINGS**

This section defines the settings for the Free flow boundary condition.

- When **No slip** is selected, the tangential component of the fluid velocity at the free-porous interface on the free-flow side (computed in the Free flow interface) is set to zero.
- When **Continuous tangential velocity** is selected, the tangential velocity component of the flow on both sides of the free-porous interface is continuous. In addition, continuity of normal stresses and conservation of mass across the interface are ensured.
- When **Beavers-Joseph** is selected, the difference of the tangential velocity components of the flow on both sides of the free-porous interface is proportional to the shear stress at the free-porous interface on the free-flow side. For this option, enter a value or expression for the **Beavers and Joseph parameter**  $a_{B,I}$  (dimensionless) that determines the proportionality. In addition, select the check box Use projected **permeability** to use only the component of the permeability tensor in the direction of the difference of the tangential velocities on both sides of the interface, instead of the trace of the permeability tensor, in determining the proportionality.
- When Beavers-loseph-Saffman is selected, the tangential velocity component of the flow at the free-porous interface on the free-flow side is proportional to the shear stress at the interface on the free-flow side. For this option also, enter a value or expression for the Beavers and Joseph parameter  $a_{RJ}$  (dimensionless) that determines the proportionality. In addition, select the check box Use projected permeability to use only the component of the permeability tensor in the direction of the difference of the tangential velocities on both sides of the interface, instead of the trace of the permeability tensor, in determining the proportionality.
- When **Viscous slip** is selected, the difference of the tangential velocity components of the flow on the free-flow side and a user-supplied interfacial velocity is proportional to the shear stress at the free-porous interface on the free-flow side. Enter values for the Slip length  $L_s$  (SI unit: m, the default is 1e-7 m), and an **Interfacial velocity u**<sub>h</sub> (SI unit: m/s, the default is 0 m/s).

In all the above cases, additionally continuity of normal stresses and conservation of mass across the interface are ensured.

Please find related information in the CFD Module User's Guide:

• The Darcy's Law Interface

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- Theory for the Darcy's Law Interface
- The Laminar Flow Interface
- Theory for the Single-Phase Flow Interfaces
- Theory for the Free and Porous Media Flow, Darcy Interface

# Chemical Species Transport Interfaces

This chapter describes the physics interfaces found under the **Chemical Species**Transport branch ( ... ). It summarizes the physics interfaces including the different fields, material properties, and boundary conditions associated with them, and suggests how and when to apply the conditions.

# 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
- The Moisture Transport Interfaces

The Moisture Flow Interface as well as The Reacting Flow in Porous Media Interface are also available under the **Chemical Species Transport** branch. They are 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 ( 1), is used to calculate the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid, or solid can be handled with this interface. The driving forces for transport can be diffusion by Fick's law, convection when coupled to a flow field, and migration, when coupled to an electric field.

The interface supports simulation of transport by convection and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration,  $c_i$ , of each species i.

#### SETTINGS

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

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

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

#### DOMAIN SELECTION

If any part of the model geometry should not partake in the mass transfer model, remove that part from the selection list.

#### **OUT-OF-PLANE THICKNESS**

For 2D components, the **Thickness** field (default value: 1 m) defines a parameter for the thickness of the geometry perpendicular to the two-dimensional cross-section. Both constant and varying thicknesses are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux.

#### CROSS-SECTIONAL AREA

For 1D components, enter a **Cross-sectional area**  $A_c$  (SI unit:  $m^2$ ) to define a parameter for the area of the geometry perpendicular to the 1D component. Both constant and varying areas are supported. The value of this parameter is used, among other things, to automatically calculate molar flow rates from the total molar flux. The default is 1  $m^2$ 

# TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the 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  $g_{lim}$ . Its defaults to 0.1[mol/m^3]/tds.helem, where tds.helem is the local element size.
- For both consistent stabilization methods, select an Equation residual. Approximate residual is the default and means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is computationally faster. If required, select **Full residual** instead.

#### INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( **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 ( **a** ) 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 ( **a**) 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 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.

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 selected. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the COMSOL Multiphysics Reference Manual.

The Value type when using splitting of complex variables setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the COMSOL Multiphysics Reference Manual.

#### **DEPENDENT VARIABLES**

The dependent variable name is the **Concentration** c by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the Number of species. Use the Add concentration (+) and Remove **concentration** ( $\equiv$ ) buttons as needed.

#### **FURTHER READING**

- Theory for the Transport of Diluted Species Interface
- Numerical Stabilization in the COMSOL Multiphysics Reference Manual.
- 2
- 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.

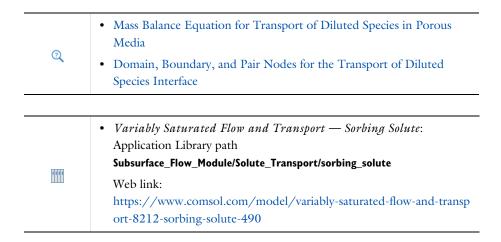
The physics interface can be used for stationary and time-dependent analysis.

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**



# 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
- Solid
- Species Properties
- 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.

# Prescribing Conditions on Fluid-Solid Interfaces

Defining conditions on interfaces between different phases, typically a wall in contact with a fluid, it is worthwhile to be careful with how variables in the conditions are evaluated. COMSOL Multiphysics supports that variables are defined differently on adjacent domains (or any other geometry dimension). Evaluating a variable with differing definitions, the mean value is returned on a boundary separating the different domains. The density, pressure, or temperature are examples of variables that may differ in a fluid and a solid. In order to specify on which side a variable is evaluated, the up and down operators (described in the COMSOL Multiphysics Reference Manual) can be used.

# Species Properties

Use this node to define parameters specific to each of the species. It is available when the Migration in electric field check box is selected in the Transport Mechanisms section of the interface.

The node will change its label depending on what inputs are available in the node. If only **Charge** is available, it will be labeled "Species charges".

#### CHARGE

Enter the charge number  $z_c$  (dimensionless, but requires a plus or minus sign) for each species.

#### ACTIVITY

This section is available when the Species Activity combo box is set to Debye-Hückel or User defined.

If **Debye-Hückel** is selected, enter the ion size number,  $a_0$ , for each species. If **User defined** is selected, enter the activity coefficient, f, for each species.

# Transport Properties

The settings in this node are dependent on the check boxes selected under Transport Mechanisms in the **Settings** window for the Transport of Diluted Species interface. It includes only the sections required by the activated transport mechanisms. It has all the equations defining transport of diluted species as well as inputs for the material properties.

#### MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the Temperature list.

#### CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the Velocity field list.

#### DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select Material, and a Fluid material to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the Fluid diffusion coefficient list.

Select Chemistry to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when Calculate transport properties is selected on the interface level of a Chemistry interface. All

defined diffusion coefficients are available for selection in the Fluid diffusion coefficient list.

For User defined, enter a value or expression for the Fluid diffusion coefficient  $D_c$  of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — Isotropic, Diagonal, Symmetric, or Full that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

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  $u_{\text{m.c.}}$ 

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**

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• 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

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• Transport in an Electrokinetic Valve: Application Library path Microfluidics\_Module/Fluid\_Flow/electrokinetic\_valve

https://www.comsol.com/model/transport-in-an-electrokinetic-valv e-603

# Solid

Use this node to describe diffusion in a solid phase domain. In this feature, the activities of the species are assumed to be ideal.

#### DIFFUSION

Specify the diffusion coefficients describing the diffusion of each species in the solid.

Enter a value or expression for the **Diffusion coefficient**  $D_c$  of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, Diagonal, or Symmetric that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

#### ADVANCED

This section is only available with the Advanced Physics Options selected and when the model contains a split between the material frame and the spatial frame. A split of these frames occurs when using a Moving Mesh node or a Structural Mechanics interface like Solid Mechanics. In such a model, the reference geometry (the material frame) differs from the deformed geometry (the spatial frame). The diffusive transport of species is solved for on the material frame, but the equation is adjusted for geometry deformations so that species conservation is achieved on the spatial frame. Use the **Diffusion model** to define the frame of reference for the diffusion tensor.

Select Reference geometry based (Lagrangian) to specify the diffusion tensor in the undeformed geometry, implying that the diffusion is defined in the material frame (indicated by coordinates X, Y, Z). This is the preferred setting for an anisotropic diffusion in combination with solid body translation or rotation. Also in general when the diffusion tensor components have been measured in an undeformed geometry.

Select Deformed geometry based (Eulerian) to specify the diffusion tensor in the deformed geometry. This means that the diffusion is defined in the spatial frame (indicated by coordinates x, y, z). Use this setting when the diffusion tensor components have been measured in a deformed geometry.

The Advanced Physics Options is found in the Show More Options dialog box, accessed by clicking the **Show More Options** button ( **5**).

Note that multiple species are only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

### Initial Values

The **Initial Values** node specifies the initial values for the concentration of each species. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

#### DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional Initial Values node.

## INITIAL VALUES

Enter a value or expression for the initial value of the **Concentration** or concentrations,  $c_i$ . This also serves as a starting guess for stationary problems.

# Mass-Based Concentrations

Use the Mass-Based Concentrations node to add postprocessing variables for mass-based concentrations (SI unit: kg/m<sup>3</sup>) 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/(m<sup>3</sup>·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 list. For an example, see the application Fine Chemical Production in a Plate Reactor as linked below.

# REACTING VOLUME

This section is only available when the Mass Transport in Porous Media property is available and selected. See https://www.comsol.com/products/specifications/ for more details on availability.

When specifying reaction rates for a species in porous media, the specified reaction rate may have the basis of the total volume, the pore volume, or in the case of using the volume of a particular phase (applicable when modeling an unsaturated porous medium).

- For **Total volume**, the reaction expressions, in  $mol/(m^3 \cdot s)$ , are specified per unit volume of the model domain (multiplied by unity).
- For **Pore volume**, the reaction expressions, in mol/(m<sup>3</sup>·s), are specified per unit volume of total pore space. The reaction expressions will be multiplied by the domain porosity,  $\varepsilon_{\rm p}$ . ( $\varepsilon_{\rm p}$  equals unity for nonporous domains).

- For Liquid phase, the reaction expressions, in mol/(m<sup>3</sup>·s), are specified per unit volume of liquid in the pore space. The expressions will be multiplied by the liquid volume fraction  $\theta_1$ . ( $\theta_1$  equals the porosity ( $\varepsilon_n$ ) on Porous Medium domains).
- For Gas phase, the reaction expressions, in mol/(m<sup>3</sup>·s), are multiplied by the gas volume fraction  $\theta_g = \epsilon_p - \theta_l$ .  $\theta_g$  equals 0 for Porous Medium domains.

# **FURTHER READING**

See the theory chapter on chemical species transport, starting with the section Mass Balance Equation.

• Fine Chemical Production in a Plate Reactor: Application Library

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

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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:

$$-\mathbf{n}\cdot(-D\nabla c-zu_{\mathbf{m}}Fc\nabla\phi)\ =\ 0$$

### CONVECTION

By default, the feature prescribes a vanishing flux due to diffusion and migration in an electric field. This is the appropriate no flux condition when the relative convective velocity at the boundary is zero. When the fluid velocity at the boundary is not equal to that of the boundary, it is often convenient to prescribe the total flux including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the no flux condition prescribed is

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = 0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathbf{m}}Fc\nabla\phi + \mathbf{u}c) = 0$$

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/m<sup>3</sup>), enter a value or expression.

# **BOUNDARY CONDITION TYPE**

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints.

The other option, Flux (Danckwerts) can be used when the concentration at the boundary is not known, or when it varies in a nontrivial manner. This may, for example, be useful when reactions with high reaction rates occur in the vicinity of the inlet. In this case the concentration far upstream of the boundary is instead prescribed. The Flux (Danckwerts) condition prescribes the total flux defined by the upstream concentration and the fluid velocity at the boundary.

### CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( ) and select **Advanced** Physics Options. You can find details about the different constraint settings in the section Constraint Reaction Terms in the COMSOL Multiphysics Reference Manual.

# **FURTHER READING**

See the theory chapter in the section Danckwerts Inflow Boundary Condition.

# Outflow

Apply this condition at outlets boundaries where species should be transported out of the model domain by fluid motion or by an electric field (in the case of ions). It is assumed that convection and migration (in an electric field) are the dominating transport mechanisms across the boundary, and therefore that the diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D\nabla c) = 0$$

Note that the Convection or the Migration in electric field transport mechanisms needs to be included for this node to be available.

# Concentration

This condition node adds a boundary condition for the species concentration. For example, a  $c = c_0$  condition specifies the concentration of species c.

### CONCENTRATION

Individually specify the concentration for each species. Select the 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.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( **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.

# 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  $\phi$ .

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

# CONVECTION

By default, the flux due to diffusion and migration in an electric field is prescribed. This is the appropriate flux condition when the relative velocity at the boundary is zero. When the fluid velocity is not equal to that of the boundary, it is often convenient to prescribe the total flux, including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the prescribed flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = J_0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathbf{m}}Fc\nabla \phi + \mathbf{u}c) = J_0$$

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:

$$-\mathbf{n} \cdot [(\mathbf{J} + \mathbf{u}c)_{11} - (\mathbf{J} + \mathbf{u}c)_{d}] = N_{0} \qquad \mathbf{J} = -D\nabla c$$

where the value  $N_0$  (SI unit: mol/(m<sup>2</sup>·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  $f(c_i)_u = f(c_i)_d$ , where  $f(c_i)_u$  is the expression enforced on the upside. Use the associated input fields to enter the upside and downside expressions for each species.

The up and downside of the selected boundary is indicated with a red arrow in the Graphics window. The arrow points from the downside into the upside. Select the Reverse direction 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.

### **BOUNDARY SELECTION**

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

### **DESTINATION SELECTION**

For more complex geometries, it might be necessary to specify the destination selection manually. To do so, right-click the Periodic Condition node and choose Manual **Destination Selection**. You can then specify the boundaries that constitute the destination surfaces in the **Destination Selection** section.

### CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button ( **5** ) and select **Advanced** Physics Options in the Show More Options dialog box. This section contains settings for specifying the type of constraint and whether to use a pointwise or weak constraint. See Constraint Settings in the COMSOL Multiphysics Reference Manual for more information.

### ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button ( **5** ) and select **Advanced** Physics Options in the Show More Options dialog box. For information about the **Orientation of Source** section, see Orientation of Source and Destination in the COMSOL Multiphysics Reference Manual.

### ORIENTATION OF DESTINATION

This section appears if the setting for Transform to intermediate map in the Orientation of Source section is changed from the default value, Automatic, and Advanced Physics **Options** is selected in the **Show More Options** dialog box. For information about the **Orientation of Destination** section, see Orientation of Source and Destination in the COMSOL Multiphysics Reference Manual.

# MAPPING BETWEEN SOURCE AND DESTINATION

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

### **FURTHER READING**

For an example of using a periodic condition, see this application example:



The KdV Equation and Solitons: Application Library path COMSOL\_Multiphysics/Equation\_Based/kdv\_equation

# Line Mass Source

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



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

### SELECTION

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

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

### SPECIES SOURCE

Enter the source strength,  $\dot{q}_{1,c}$ , 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.

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



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

### SPECIES SOURCE

Enter the source strength,  $\dot{q}_{\rm p,c}$ , 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

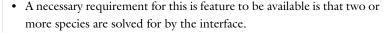
This feature models a thin mass transfer barrier. It is available on interior boundaries and introduces a discontinuity in the concentration across the boundary. On each side, a no-flux condition is prescribed for the mass transport implying that it acts as a barrier. The feature can be used to avoid 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  $R_{
m eq}$ ) 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.





• 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**  $K_{eq}$  (dimensionless). Also enter a value or expression for the **Unit activity concentration**  $C_{a0}$  (SI unit: mol/m<sup>3</sup>). 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  $E_{\mathrm{eq}}$  (dimensionless).

### STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient  $\nu_c$  (dimensionless). The default is 0. Use negative values for reactants and positive values for products in the modeled reaction.

Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium** Reaction node.

# Surface Reactions

The Surface Reactions node can be used to account for the species boundary flux due to chemical reactions occurring on a surface (heterogeneous reactions). For a domain species participating in a surface reaction, the boundary flux corresponds to the reaction rate at the surface.

# SURFACE REACTION RATE

Specify the surface reaction rate  $J_0$  of each species resulting from the reactions. Note that if you have the Chemistry interface available, provided with the Chemical Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down list.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.

# **FURTHER READING**

For an example of using the Surface Reactions node, see this application example:



Chemical Vapor Deposition of GaAs: Application Library path

Chemical\_Reaction\_Engineering\_Module/Reactors\_with\_Mass\_and\_Heat\_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.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

# Fast Irreversible Surface Reaction

This boundary node defines an irreversible reaction where the kinetics is so fast that the only factor limiting the reaction rate is the transport of a species to the reacting surface.

The node will set the Rate limiting species concentration to zero at the boundary, and balance the fluxes of the species participating in the reaction and the current densities according to the Stoichiometric Coefficients settings.

When defining conditions on boundaries between different phases, see the section Prescribing Conditions on Fluid-Solid Interfaces.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

# Porous Electrode Coupling

Use this node to add a molar source in a domain that is coupled to one or multiple Porous Electrode Reaction nodes of an Electrochemistry Interface.

The molar source is calculated from the number of electrons, stoichiometric coefficients, and volumetric current densities of the coupled porous electrode reactions specified in the **Reaction Coefficients** subnodes.

In the Transport of Concentrated Species interface, the molar sources (or sinks) are multiplied by the species molar masses to obtain the corresponding mass sources.

Additional Reaction Coefficients subnodes are available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass source or sink, which is often the case in gas diffusion electrodes, you need to also add a corresponding 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/m<sup>2</sup>) 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  $\boldsymbol{n}_m$  (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.

# Fluid

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  $D_{\rm F\,i}$  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  $\tau_{\rm Fi}$  (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  $u_{me}$  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  $\textbf{Porosity}\; \boldsymbol{\epsilon}_{p}$  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  $\rho_b$  and the (single phase) Pellet density  $\rho_{pe}$ . The porosity is then defined from

$$\varepsilon_{p} = 1 - \frac{\rho_{b}}{\rho_{pe}}$$

For **User defined**, enter a value or expression for the porosity.

# Dispersion

Local variations in the velocity as the fluid flows around solid particles lead to mechanical mixing, referred to as dispersion. Use this feature to account for dispersion in a Porous Medium or a Unsaturated Porous Medium

This subfeature is available when both the Mass transfer in porous media mass transfer check box and the Convection check box are selected in 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: m<sup>2</sup>/s) for each species separately. When not selected the same dispersion tensor  $D_D$  is used for all species.

Select an option from the Dispersion tensor list — Dispersivity or User defined.

Select **Dispersivity** to specify the dispersion in terms of dispersivities (SI unit: m). Select an option from the Dispersivity model list: Isotropic (the default) or Transverse isotropic based on the properties of the porous media. For isotropic porous media, specify the longitudinal and transverse dispersivities. For transverse isotropic porous media, specify the longitudinal, horizontal transverse, and vertical transverse dispersivities.

For **User defined**, specify the dispersion components in terms of constants or expressions. Select Isotropic, Diagonal, Symmetric, or Full to enable the appropriate tensor components.

# Unsaturated Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

Use this node to model the concentration of diluted species transported by a liquid (mobile fluid phase) in a partially filled solid porous medium. The interstices of the porous medium contains the liquid carrier phase and gas pockets. Apart from

convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and volatilization.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The properties of each phase present are defined using the Liquid, the Gas, and the Porous Matrix subnodes respectively. The Unsaturated Porous Medium node supports material properties using a Porous Material node (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  $\theta_{l} = \varepsilon_{p} s$ .

For **Liquid volume fraction**, enter a value for  $\theta_1$  (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**  $C_{\rm m}$  (SI unit:  $1/{\rm m}$ ). 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  $D_{L,i}$  of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an Effective diffusivity model, liquid to account for the reduced diffusivity in the liquid. The available models are Millington and Quirk model

(the default), Bruggeman model, Tortuosity model, or No correction. For Tortuosity **model**, enter a value for the tortuosity  $\tau_{L,i}$  (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. For details see: https://www.comsol.com/products/specifications/.

### MIGRATION IN ELECTRIC FIELD

This section is available when the Migration in electric field 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.

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**  $\rho$ , or the **Solid phase density**  $\rho_s$ . 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: m<sup>3</sup>/mol) and an Adsorption maximum  $c_{p,\text{max,c}}$  (SI unit: mol/kg).

• For Freundlich:

$$c_{\rm P} = K_{\rm F} \left(\frac{c}{c_{\rm ref}}\right)^N$$
 ,  $K_P = \frac{\partial c_{\rm P}}{\partial c} = N \frac{c_{\rm P}}{c}$ 

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/m<sup>3</sup>).

• 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

$$K_P = \frac{\partial c_P}{\partial c} = c_{\text{Pmax}} b_{\text{T}} (1 + (b_{\text{T}} c)^{N_{\text{T}}})^{-\left(1 + \frac{1}{N_{\text{T}}}\right)}$$

Enter a **Toth constant**  $b_{T,c}$  (SI unit: m<sup>3</sup>/mol), a **Toth exponent**  $N_{T,c}$  (dimensionless), and an Adsorption maximum  $c_{p,max,c}$  (SI unit: mol/kg).

• For BET (Brunauer-Emmett-Teller):

$$c_{\rm P} = \frac{K_{\rm B} c_0 c}{(c_{\rm S} - c) \left(1 + (K_{\rm B} - 1) \frac{c}{c_{\rm S}}\right)}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = \frac{K_B c_0 c_S ((K_B - 1)c^2 + c_S^2)}{(c - c_S)^2 (c_S + (K_B - 1)c)^2}$$

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/m<sup>3</sup>).

• For User defined enter an Adsorption isotherm  $c_{P,c}$  (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.

This feature is available when the **Mass transfer in porous media** check box is selected in the **Settings** window for the physics interface.

Use this feature to model mass transfer at the boundary due to volatilization. The species dissolved in the liquid are assumed to be vaporized at the boundary, and transported into the surrounding bulk region due to convection and diffusion. The mass transfer at the boundary is defined as

$$-\mathbf{n} \cdot \mathbf{J}_{c} = -h_{c}(k_{G,c}c - c_{Gatm,c})$$

where  $h_c$  is the mass transfer coefficient,  $k_{G,c}$  the volatilization coefficient, and  $c_{\text{Gatm.c}}$ 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  $D_{
m Gc}$  and the thickness of the diffusion layer  $d_{
m s}$  in the manner of

$$h_{\rm c} = \frac{D_{Gc}}{d_{\rm s}}$$

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.

# Species Source

In order to account for consumption or production of species in porous domains, the **Species Source** node adds source terms expressions  $S_i$  to the right-hand side of the species transport equations.

### DOMAIN SELECTION

From the Selection list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

If there are several types of domains, with subsequent and different reactions occurring within them, it might be necessary to remove some domains from the selection. These are then defined in an additional Species Source node.

### SPECIES SOURCE

Add a source term  $S_i$  (SI unit: mol/(m<sup>3</sup>·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  $c_{\text{mo,ref}}$  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.

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 5-1 shows examples of possible situations in which this type of geometry reduction can be applied.

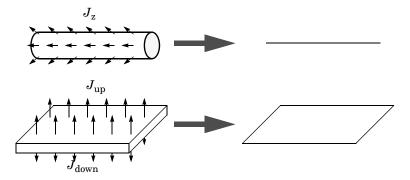


Figure 5-1: Geometry reduction from 3D to 1D (top) and from 3D to 2D (bottom).

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, the mass transfer of species i is defined by the mass conservation equation

$$\frac{\partial c_{i}}{\partial t} + \nabla \cdot \mathbf{J}_{i} + \mathbf{u} \cdot \nabla c_{i} = R_{i} + S_{\mathbf{opf}, i}, \qquad (5-1)$$

where  $S_{\text{opf},i}$  is the out-of-plane source for species i

$$S_{\mathrm{opf},i} = \frac{J_{0,i}}{d_z} = \frac{J_{0,u,i} + J_{0,d,i}}{d_z}.$$

For external convection on the upside and the downside of the domain, the out-of-plane flux is

$$J_{0,i} = k_{c,u,i}(c_{b,u,i} - c_i) + k_{c,d,i}(c_{b,d,i} - c_i)$$

where  $k_c$  is a mass transfer coefficient and  $c_b$  is the bulk concentration, the typical concentration far into the surrounding exterior domain. The prescribed flux,  $J_0$ , can include any arbitrary user-specified expressions. It can be a constant or a function of a dependent variable or independent variables.

# UPSIDE INWARD FLUX

For 1D components, enter the cross-sectional perimeter Pc 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.

The Fracture feature has two default subfeatures — the Fluid (Fracture) subfeature where convection and diffusion are specified and the Fracture Material subfeature where the porosity  $\varepsilon_{p}$  is defined.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

### FRACTURE PROPERTIES

Specify a value for the **Fracture thickness**  $d_{\rm fr}$ .

For the Fracture boundary condition, there are a number of Attributes available which can be accessed either via the Physics Ribbon toolbar (for Windows) or by right-clicking on the **Fracture** node. These attributes are identical to the Boundary, Edge, Point, and Pair Nodes for the Transport of Diluted Species in Fractures Interface.

# Fluid (Fracture)

Use this node to specify the mass transfer in the mobile fluid solvent filling the pores of a fracture.

It uses the same input options as the Fluid subfeature under the Porous Medium feature. There are further details about the settings.

### MODEL INPUTS

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

# CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use a Fracture feature in a Darcy's Law interface to compute the fluid flow velocity in the fracture.

For **User defined**, enter values or expressions for the velocity components in the table shown

# DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.



The **Diffusion** settings are similar to those for the diffusion coefficients in the Fluid node under Porous Medium.

# Fracture Material

Specify the **Porosity,**  $\varepsilon_{\rm p}$  (dimensionless) of the porous matrix. This is by default taken From material. Select From pellet bed densities to compute the porosity from the (dry bulk) Bed density  $\rho_b$  and the (single phase) Pellet density  $\rho_{pe}$  through the relation

$$\varepsilon_{\rm p} = 1 - \frac{\rho_{\rm b}}{\rho_{\rm pe}}$$

For **User defined**, enter a value or expression for the porosity.

# The Transport of Diluted Species in Fractures Interface

The Transport of Diluted Species in Fractures (dsf) interface (17), 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 the model geometry includes boundaries that should not be included in the mass transfer simulation, remove those 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.

### TRANSPORT MECHANISMS

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 ( **a** ) 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  $g_{lim}$ . Its default value is 0.1[mol/m<sup>3</sup>)/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.

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- 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).

- Concentration
- Flux
- Fracture
- Inflow
- Initial Values

- No Flux
- Outflow
- · Reactions
- · Species Source

Furthermore, there are the following attributes to the Fracture node

- Adsorption
- Dispersion

# Adsorption

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 **Boundary material** is used as The Transport of Diluted Species in Fractures Interface is active on boundaries only. The **Density**  $\rho$  of the porous media is needed when modeling adsorption to the surface of the porous matrix. By default the option From material is selected.

# 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). Also activate the check box for the species  $c_i$ for which adsorption takes place.

• For Langmuir:

$$c_{\mathrm{P}} = c_{\mathrm{Pmax}} \frac{K_{\mathrm{L}}c}{1 + K_{\mathrm{L}}c} \quad \frac{\partial c_{\mathrm{P}}}{\partial c} = \frac{K_{\mathrm{L}}c_{\mathrm{Pmax}}}{(1 + K_{\mathrm{L}}c)^2}$$

Enter a Langmuir constant  $k_{L,c}$  (SI unit: m<sup>3</sup>/mol) and an Adsorption maximum  $c_{p,\text{max.c}}$  (SI unit: mol/kg):

• For Freundlich:

$$c_{\rm P} = K_{\rm F} \left(\frac{c}{c_{\rm ref}}\right)^N \frac{\partial c_{\rm P}}{\partial c} = N \frac{c_{\rm P}}{c}$$
 Freundlich

Enter a Freundlich constant  $k_{
m F,c}$  (SI unit: mol/kg), a Freundlich exponent  $N_{
m F,c}$ (dimensionless), and a Reference concentration  $c_{\rm ref,c}$  (SI unit: mol/m<sup>3</sup>).

• 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

$$\frac{\partial c_{\mathrm{P}}}{\partial c} = c_{\mathrm{Pmax}} b_{\mathrm{T}} (1 + (b_{\mathrm{T}} c)^{N_{\mathrm{T}}})^{-\left(1 + \frac{1}{N_{\mathrm{T}}}\right)}$$

Enter a **Toth constant**  $b_{T,c}$  (SI unit: m<sup>3</sup>/mol), a **Toth exponent**  $N_{T,c}$  (dimensionless), and an Adsorption maximum  $c_{p,\max,c}$  (SI unit: mol/kg).

• For BET (Brunauer-Emmett-Teller):

$$c_{\rm P} = \frac{K_{\rm B} c_0 c}{(c_{\rm S} - c) \left(1 + (K_{\rm B} - 1) \frac{c}{c_{\rm S}}\right)}$$

and

$$\frac{K_{\rm B}c_0c_{\rm S}((K_{\rm B}-1)c^2+c_{\rm S}^2)}{(c-c_{\rm S})^2(c_{\rm S}+(K_{\rm B}-1)c)^2}$$

Enter a BET constant  $K_{\mathrm{B,c}}$  (dimensionless), a Monolayer adsorption capacity  $c_{0,\mathrm{c}}$ (SI unit: mol/kg), and a **Saturation concentration**  $c_{S,c}$  (SI unit: mol/m<sup>3</sup>).

For User defined:

$$c_{\rm p} = f(c)$$

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 ( **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.

# 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 Fracture.

This subfeature is available when the Convection check box is selected in 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: m<sup>2</sup>/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.

# 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

$$\mathbf{n} \cdot d_{\mathrm{fr}}(D_{\mathrm{e}} \nabla c) = d_{\mathrm{fr}} N_{\mathrm{o}}$$

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

The available options are **General inward flux** and **External convection**. If the latter is chosen, define a Mass transfer coefficient and a Bulk concentration. Specify the flux of each species individually. To use another boundary condition for a specific species, make sure that the check box for the mass fraction of that species is unchecked.

# 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  $e_{0,c}$  (SI unit: mol/m<sup>3</sup>), 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 ( **3**) 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 list.

## 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  $d_{\mathrm{fr}}$ .
- For **Pore volume**, the reaction expressions in mol/(m<sup>3</sup>·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 low compared to a solvent fluid or solid. As a rule of thumb, a mixture containing several species can be considered dilute when the concentration of the solvent is more than 90 mol%. Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent.

When studying mixtures that are not dilute, the mixture and transport properties depend on the composition, and a different physics interface is recommended. See The Transport of Concentrated Species Interface in the Chemical Reaction Engineering Module User's Guide for more information.

Fick's law governs the diffusion of the solutes, dilute mixtures, or solutions, while the phenomenon of ionic migration is sometimes referred to as electrokinetic flow. The Transport of Diluted Species interface supports the simulations of chemical species transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D.

### In this section:

- Adding Transport Through Migration
- 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:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i \tag{5-2}$$

Equation 5-2 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/m<sup>3</sup>)
- $D_i$  denotes the diffusion coefficient (SI unit:  $m^2/s$ )
- $R_i$  is a reaction rate expression for the species (SI unit: mol/(m<sup>3</sup>·s))
- **u** is the mass averaged velocity vector (SI unit: m/s)
- $J_i$  is the mass flux diffusive flux vector (SI unit: mol/(m<sup>2</sup>·s))

The mass flux relative to the mass averaged velocity,  $\mathbf{J}_i$  (SI unit: mol/(m<sup>2</sup>·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  $J_i$  defines the diffusive flux vector

$$\mathbf{J}_i = -D\nabla c_i \tag{5-3}$$

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 5-2 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 5-2),  $R_i$  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:

$$K_{\text{eq}} = \frac{\prod_{i \in \text{products}} a_i^{v_i}}{\prod_{i \in \text{reactants}} a_i^{-v_i}}$$

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:

$$K_{\text{eq}} = \prod_{i} a_{i}^{v_{i}}$$

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 in the Settings window. For nonunity activity coefficients, a user defined equilibrium condition can be used.

## EQUILIBRIUM REACTIONS AND INFLOW BOUNDARY CONDITIONS

Contradictory constraints arise if the boundary conditions for concentrations or activities are set so that the domain equilibrium condition is not fulfilled. Special treatment is therefore needed at Inflow boundaries, where the concentrations are set for all species in the mass transport interfaces.

One way of avoiding competing constraints on an inflow boundary is to add an additional reaction coordinate degree of freedom, solved for to create a set of modified inflow concentrations that fulfill the domain equilibrium condition. The reaction coordinate gives rise to a concentration shift, which is the offset to the inflow concentrations provided by the user. The shift for each species obeys the stoichiometry of the reaction and the equilibrium expression. The modified inflow concentrations are then used in the boundary conditions for the domain mass transport equations. The resulting modified inflow concentrations can be seen as the stationary solution for a batch reactor with the user inflow concentrations as initial concentrations. In addition, the domain reaction rate degree of freedom of the equilibrium reaction is constrained to zero on all Inflow boundaries.

# 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 5-2.

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: 
$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot \mathbf{J}_i + R$$
 (5-4)

conservative: 
$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}) = \nabla \cdot \mathbf{J}_i + R$$
 (5-5)

and each is treated slightly differently by the solver algorithms. In these equations  $J_i$  (SI unit: mol/(m<sup>2</sup>·s)) is the diffusive flux vector, R (SI unit: mol/(m<sup>3</sup>·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 ( **a** ) and select Advanced Physics Options.

Remove the convection term from Equation 5-4 and Equation 5-5 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,  $Q_{\rm c}$  (SI unit: mol/(m<sup>3</sup>·s)), in a small volume  $\delta V$  and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength,  $\dot{q}_{\mathrm{p,c}}$ (SI unit: mol/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{SV} Q_{c} = \dot{q}_{p,c} \tag{5-6}$$

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 5-6,  $Q_{
m c}$  must tend to plus or minus infinity as  $\delta V$  tends to zero. This means that in theory the concentration also tends to plus or minus infinity.

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

The finite element representation of Equation 5-6 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  $Q_{1,c}$  (SI unit: mol/(m<sup>3</sup>·s)), located within a tube with cross section  $\delta S$  and then letting  $\delta S$  tend to zero while keeping the total mass flux per unit length constant. Given a line source strength,  $\dot{q}_{1,c}$  (SI unit: mol/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} Q_{l,c} = q_{l,c} \tag{5-7}$$

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

$$q_{l,c}$$
test $(c)$ 

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

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

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For feature node information, see Line Mass Source and Point Mass Source.

**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:

$$\frac{\partial c_{i}}{\partial t} + \nabla \cdot (-D_{i} \nabla c_{i} - z_{i} u_{m,i} F c_{i} \nabla V + c_{i} \mathbf{u}) = R_{i}$$
 (5-8)

where

- $c_i$  (SI unit: mol/m<sup>3</sup>) denotes the concentration of species i
- $D_i$  (SI unit: m<sup>2</sup>/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
- $u_{\text{m }i}$  (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 electroactive species. This also means that the concentration gradients of the predominant species in a supporting electrolyte are usually negligible.

Modeling and solving for a supporting electrolyte in the *Electrostatics* or *Secondary* Current Distribution interfaces will give a potential distribution that drives the migration in the Transport of Diluted Species Interface.

The current density vector is proportional to the sum of all species fluxes as expressed by Faraday's law:

$$\mathbf{i} = F \sum_{i} z_{i} \mathbf{N}_{i}$$

The electroneutrality condition ensures that there is always a zero net charge at any position in a dilute solution. Intuitively, this means that it is impossible to create a current by manually pumping positive ions in one direction and negative ions in the other. Therefore, the convective term is canceled out to yield the following expression for the electrolyte current density, where j denotes the supporting species:

$$\mathbf{i} = F \sum_{j} -z_{j}^{2} u_{\mathrm{m},j} F c_{j} \nabla \phi \tag{5-9}$$

Equation 5-9 is simply Ohm's law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa \nabla \phi \tag{5-10}$$

where  $\kappa$  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 5-10, yields:

$$\nabla \cdot (-\kappa \nabla \phi) = 0 \tag{5-11}$$

Equation 5-11 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 Péclet number — that is, systems where convection or migration dominates over diffusion. Streamline diffusion and crosswind diffusion are of paramount importance to obtain physically reasonable results. The Transport of Diluted Species interface provides two crosswind diffusion options using different formulations. Observe that crosswind diffusion makes the equation system nonlinear even if the transport equation is linear.

### DO CARMO AND GALEÃO

This is the formulation described in Numerical Stabilization in the COMSOL Multiphysics Reference Manual. The method reduces over- and undershoots to a minimum, even for anisotropic meshes.

In some cases, the resulting nonlinear equation system can be difficult to converge. This can happen when the cell Péclet number is very high and the model contains many thin layers, such as contact discontinuities. You then have three options:

- Refine the mesh, especially in regions with thin layers.
- Use a nonlinear solver with a constant damping factor less than one.
- Switch to the Codina crosswind formulation.

## CODINA

The Codina formulation is described in Ref. 1. It adds diffusion strictly in the direction orthogonal to the streamline direction. Compared to the do Carmo and Galeão formulation, the Codina formulation adds less diffusion but is not as efficient at reducing over- and undershoots. It also does not work as well for anisotropic meshes. The advantage is that the resulting nonlinear system is easier to converge and that underresolved gradients are less smeared out.

# Danckwerts Inflow Boundary Condition

Constraining the composition to fixed values at an inlet to a reactor may sometimes result in issues with unreasonably high reaction rates or singularities at the inlet boundary. These problems may many times be mitigated by using a flux boundary condition instead, based on the upstream concentrations and the fluid velocity at the boundary. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet conditions for domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an upstream concentration  $c_{i,0}$ , the Danckwerts inflow boundary condition prescribed the total flux as

$$\mathbf{n} \cdot (\mathbf{J}_i + \mathbf{u}c_i) = \mathbf{n} \cdot (\mathbf{u}c_{i,\,0}) \tag{5-12}$$

### 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:

$$\begin{split} \frac{\partial}{\partial t}(\theta_{\text{I}}c_{i}) + \frac{\partial}{\partial t}(\rho c_{\text{P},\,i}) + \frac{\partial}{\partial t}(\theta_{\text{g}}c_{\text{G},\,i}) + \mathbf{u} \cdot \nabla c_{i} &= \\ \nabla \cdot \left[ (D_{\text{D},\,i} + D_{\text{e},\,i}) \nabla c_{i} \right] + R_{i} + S_{i} \end{split} \tag{5-13}$$

On the left-hand side of Equation 5-13, 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 **u** (SI unit: m/s).

In Equation 5-13  $c_i$  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  $\varepsilon_p$ , the liquid volume fraction  $\theta_l$ ; the dry bulk density,  $\rho = (1 - \varepsilon_s)\rho_s$ , and the solid phase density  $\rho_s$ .

For saturated porous media, the liquid volume fraction  $\theta_l$  is equal to the porosity  $\epsilon_p$ , but for unsaturated porous media, they are related by the saturation s as  $\theta_l = \epsilon_p s$ . 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 5-13, 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: m<sup>2</sup>/s) and the effective diffusion by  $D_{\rm e}$  (SI unit: m<sup>2</sup>/s).

The last two terms on the right-hand side of Equation 5-13 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

$$\frac{\partial}{\partial t}(\rho c_{P,i}) = \rho \frac{\partial c_{P,i}}{\partial c_i} \frac{\partial c_i}{\partial t} - c_{P,i} \rho_s \frac{\partial \varepsilon_P}{\partial t} = \rho K_{P,i} \frac{\partial c_i}{\partial t} - c_{P,i} \rho_s \frac{\partial \varepsilon_P}{\partial t}$$
 (5-14)

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

$$\frac{\partial}{\partial t} \theta_{g} c_{G,i} = \theta_{g} \frac{\partial c_{G,i}}{\partial c_{i}} \frac{\partial c_{i}}{\partial t} + k_{G,i} c_{i} \frac{\partial \theta}{\partial t}^{g} = \theta_{g} k_{G,i} \frac{\partial c_{i}}{\partial t} + k_{G,i} c_{i} \frac{\partial \theta}{\partial t}^{g}$$
(5-15)

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

$$\frac{\partial}{\partial t} (\varepsilon_{\mathbf{p}} c_i) + \frac{\partial}{\partial t} (\rho c_{\mathbf{P}, i}) + \mathbf{u} \cdot \nabla c_i = \nabla \cdot [(D_{\mathbf{D}, i} + D_{\mathbf{e}, i}) \nabla c_i] + R_i + S_i$$
 (5-16)

# 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:

$$\mathbf{u}_{a} = \frac{\mathbf{u}}{\varepsilon_{p}}$$
 Saturated

$$\mathbf{u}_{a} = \frac{\mathbf{u}}{\varepsilon_{p}}$$
 Saturated  $\mathbf{u}_{a} = \frac{\mathbf{u}}{\theta_{1}}$  Unsaturated

where  $\varepsilon_{\rm p}$  is the porosity and  $\theta_{\rm l}$  =  $s\varepsilon_{\rm p}$  the liquid volume fraction, and s the saturation, a dimensionless number between 0 and 1.



Figure 5-2: 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 5-13 is written as:

$$\begin{split} \frac{\partial}{\partial t}(\theta_{\text{I}}c_{i}) + \frac{\partial}{\partial t}(\rho c_{\text{P},\,i}) + \frac{\partial}{\partial t}(\theta_{g}c_{\text{G},\,i}) + \nabla \cdot \mathbf{u}c_{i} &= \\ \nabla \cdot [(D_{\text{D},\,i} + D_{\text{e},\,i})\nabla c_{i}] + R_{i} + S_{i} \end{split} \tag{5-17}$$

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 5-13.

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 or in 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  $D_{\rm F}$ ,  $D_{\rm L}$ , and  $D_{\rm G}$  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  $\tau_F$ ,  $\tau_L$ , and  $\tau_G$  are the corresponding tortuosity factors (dimensionless).

The tortuosity factor accounts for the reduced diffusivity due to the fact that the solid grains impede Brownian motion. The interface provides predefined expressions to

compute the tortuosity factors in partially saturated porous media according to the Millington and Quirk model (Ref. 3):

$$\tau_L = \theta_l^{-7/3} \varepsilon_p^2, \tau_G = \theta_g^{-7/3} \varepsilon_p^2$$

and Bruggeman model

$$\tau_L = \theta_l^{-5/2} \varepsilon_p^2, \tau_G = \theta_g^{-5/2} \varepsilon_p^2$$

For saturated porous media  $\theta_l = \epsilon_p$ . 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 low.

The spreading of mass, as a fluid travel through a porous medium is caused by several contributing effects. Local variations in fluid velocity lead to mechanical mixing referred to as dispersion occurs because the fluid in the pore space flows around solid particles, so the velocity field varies within pore channels. The spreading in the direction parallel to the flow, or longitudinal dispersivity, typically exceeds the transverse dispersivity from up to an order of magnitude. Being driven by the concentration gradient alone, molecular diffusion rate is low relative to the mechanical dispersion, except at very low fluid velocities.

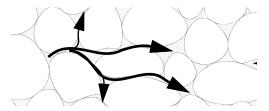


Figure 5-3: Spreading of fluid around solid particles in a porous medium.

The dispersion is controlled through the dispersion tensor  $D_{\rm D}$ . The tensor components can either be given by user-defined values or expressions or derived from the directional dispersivities.

Using the longitudinal and transverse dispersivities in 2D, the dispersivity tensor components are (Ref. 5):

$$D_{\mathrm{D}ii} = \alpha_{\mathrm{L}} \frac{u_i^2}{|\mathbf{u}|} + \alpha_{\mathrm{T}} \frac{u_j^2}{|\mathbf{u}|}$$

$$D_{\mathrm{D}ij} = D_{\mathrm{D}ji} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}}) \frac{u_i u_j}{|\mathbf{u}|}$$

In these equations,  $D_{Dii}$  (SI unit: m<sup>2</sup>/s) are the principal components of the dispersivity tensor, and  $D_{\mathrm{D}ji}$  and  $D_{\mathrm{D}ji}$  are the cross terms. The parameters  $\alpha_{\mathrm{L}}$  and  $\alpha_{\mathrm{T}}$ (SI unit: m) specify the longitudinal and transverse dispersivities; and  $u_i$  (SI unit: m/s) stands for the velocity field components.

In order to facilitate modeling of stratified porous media in 3D, the tensor formulation by Burnett and Frind (Ref. 4) can be used. Consider a transverse isotropic media, where the strata are piled up in the z direction, the dispersivity tensor components are:

$$\begin{split} D_{\text{L}xx} &= \alpha_{1} \frac{u^{2}}{|\mathbf{u}|} + \alpha_{2} \frac{v^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{w^{2}}{|\mathbf{u}|} \\ D_{\text{L}yy} &= \alpha_{1} \frac{v^{2}}{|\mathbf{u}|} + \alpha_{2} \frac{u^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{w^{2}}{|\mathbf{u}|} \\ D_{\text{L}zz} &= \alpha_{1} \frac{w^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{u^{2}}{|\mathbf{u}|} + \alpha_{3} \frac{v^{2}}{|\mathbf{u}|} \\ D_{\text{L}xy} &= D_{\text{L}yx} = (\alpha_{1} - \alpha_{2}) \frac{uv}{|\mathbf{u}|} \\ D_{\text{L}xz} &= D_{\text{L}zx} = (\alpha_{1} - \alpha_{3}) \frac{uw}{|\mathbf{u}|} \\ D_{\text{L}yz} &= D_{\text{L}zy} = (\alpha_{1} - \alpha_{3}) \frac{vw}{|\mathbf{u}|} \end{split}$$

In Equation 5-18 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  $\alpha_1$  (SI unit: m) is the longitudinal dispersivity. If z is the vertical axis,  $\alpha_2$  and  $\alpha_3$  are the dispersivities in the transverse horizontal and transverse vertical directions, respectively (SI unit: m). Setting  $\alpha_2 = \alpha_3$  gives the expressions for isotropic media shown in Bear (Ref. 5 and Ref. 6).

# Adsorption

As species travel through a porous medium they typically attach to (adsorb), and detach (desorb) from the solid phase, which slows chemical transport through the porous medium. Adsorption and desorption respectively reduces or increases species concentrations in the fluid. The adsorption properties vary between chemicals, so a plume containing multiple species can separate into components (Ref. 7). The Adsorption feature includes four predefined and one user defined relationships to predict the solid concentrations,  $c_{Pi}$  from the concentration in the liquid phase,  $c_i$ :

$$c_{\rm P} = c_{\rm Pmax} \frac{K_{\rm L}c}{1 + K_{\rm L}c}$$
 Langmuir 
$$c_{\rm P} = K_{\rm F} \left(\frac{c}{c_{\rm ref}}\right)^{N}$$
 Freundlich 
$$c_{\rm P} = c_{\rm Pmax} \frac{b_{\rm T}c}{\left(1 + \left(b_{\rm T}c\right)^{N_{\rm T}}\right)^{1/N_{\rm T}}}$$
 Toth 
$$c_{\rm P} = \frac{K_{\rm B}c_{\rm 0}c}{(c_{\rm S} - c)\left(1 + \left(K_{\rm B} - 1\right)\frac{c}{c_{\rm S}}\right)}$$
 BET

The above equations contains the following parameters:

- Freundlich (Ref. 8)
  - Freundlich constant  $K_{
    m F}$  (SI unit:·mol/kg), Freundlich exponent  $N_{
    m F}$ (dimensionless), and reference concentration  $c_{ref}$  (SI unit: mol/m<sup>3</sup>).
- Langmuir (Ref. 9)
  - Langmuir constant  $K_{\rm L}$  (SI unit: m<sup>3</sup>/mol), and adsorption maximum  $c_{\rm Pmax}$ (SI unit: mol/kg).
- Toth (Ref. 10)
  - Toth constant  $b_{\rm T}$  (SI unit: m<sup>3</sup>/mol), Toth exponent  $N_{\rm T}$  (dimensionless), and adsorption maximum  $c_{\mathrm{Pmax}}$  (SI unit: mol/kg).
- BET (Brunauer–Emmett–Teller, Ref. 11)
  - BET constant  $K_{
    m B}$  (dimensionless), the monolayer adsorption capacity  $c_0$ (SI unit: mol/kg) and the saturation concentration,  $c_S$  (SI unit: mol/m<sup>3</sup>).

These predefined expressions are adsorption isotherms that describe the amount of species sorbed to the solid. Applying the isotherms, as defined in the Adsorption section above, assumes that adsorption is at equilibrium locally. This implies that the species phase transfer, between the fluid and the solid phase (within the porous medium), is much faster than the transport within the fluid phase.

Using a Species Source feature, arbitrary expressions can be entered to define, for example, nonequilibrium and temperature-dependent adsorption laws, in the manner of Fetter (Ref. 12), or Bear and Verruijt (Ref. 13).

The retardation factor, RF, describes how adsorption slows the solute velocity,  $\mathbf{u}_c$ , relative to the average linear velocity of the fluid,  $\mathbf{u}_a$ , as in

$$RF = 1 + \frac{\rho_b}{\theta} \frac{\partial c_P}{\partial c} = \frac{\mathbf{u}_a}{\mathbf{u}_c}$$

If the contaminant moves at the average linear velocity of the fluid for RF = 1. For RF > 1, the contaminant velocity is lower than the fluid velocity owing to residence time on solids.

## Reactions

Chemical reactions of all types influence species transport in porous media. Examples include biodegradation, radioactive decay, transformation to tracked products, temperature- and pressure-dependent functions, exothermic reactions, and endothermic reactions. The reactions represent change in species concentration per unit volume porous medium per time. Reaction terms are used on the right-hand side of the governing equation to represent these processes. For reactions in a fluid phase, multiply the expression by the fluid volume fraction  $\theta$ . Similarly, solid phase reaction expressions include the bulk density,  $\rho_b$ , 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  $\lambda$  is the chemical half life,  $\zeta$  is a reaction rate, and the subscripts L, P, and G denote liquid, solid, and gas phases, respectively. In the equations, the reactions either depend on liquid concentration  $c_i$  or solid phase concentrations  $c_{Pi}$  obtained using the sorption derivative with  $c_i$  or gas phase concentration  $c_{Gi}$  depending on the gas volume fraction, the volatilization, and the liquid concentration.

Reaction rates can vary with results from other equations in your model, such as temperature. For example, enter the Arrhenius rate law given in Ref. 14:

$$\zeta_T = \zeta_R \exp\left[\frac{E_a(T - T_R)}{R_u T T_R}\right]$$
 (5-20)

In Equation 5-20, 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,  $\kappa$  is the fracture permeability,  $\mu$  the fluid's dynamic viscosity, and  $\nabla_t p$  is the tangential gradient of the fluid pressure.

The equation to solve for mass transport of species  $c_i$  in a thin fracture, embedded in a porous media, is derived from Equation 5-13. The resulting equation is:

$$d_{\text{fr}} \left( \frac{\partial \rho_{\text{b}} c_{\text{P},i}}{\partial t} + \frac{\partial \varepsilon_{\text{p}} c_{i}}{\partial t} + \nabla_{\text{t}} \cdot (D_{\text{e},i} \nabla_{\text{t}} c_{i}) + \mathbf{u} \cdot \nabla_{\text{t}} c_{i} \right) = d_{\text{fr}} R_{i} + d_{\text{fr}} S_{i} + n_{0} \quad (5-21)$$

Here  $d_{fr}$  is the fracture thickness,  $c_{P,i}$  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:

$$\nabla c_i = \nabla_t c_i$$

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.

2

See Fracture for more information about the boundary feature solving Equation 5-21. 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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# The Moisture Transport Interfaces

The Moisture Transport interfaces available under the Chemical Species Transport branch are used to model moisture transport in porous media and building materials (by taking into account moisture storage and liquid transport by capillary suction forces) and in moist air (by convection and diffusion of vapor in moist air).

The following interfaces and features are described in the Heat Transfer Module User's Guide:

- The Moisture Transport in Air Interface
- The Moisture Transport in Porous Media Interface
- The Moisture Transport in Building Materials Interface
- The Moisture Transport Features
- Theory for Moisture Transport

In this manual you find:

- The Moisture Transport in Solids Interface
- Theory for Moisture Transport in Solids

# The Moisture Transport in Solids Interface

The Moisture Transport in Solids (mts) interface ( No ), found under the Chemical Species **Transport** branch ( is used to model moisture diffusion in a solid.



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

The interface supports simulation of moisture transport by diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The default unit of the dependent variables are the relative humidity and moist air pressure.

When this physics interface is added, these default nodes are also added to the Model Builder: **Porous Medium**, **No Flux** (prescribing no moisture flux across all external boundaries on which no other boundary condition has been specified), and **Initial** Values. Then, from the Physics toolbar, you can add other nodes that implement, for example, boundary conditions and source terms. You can also right-click Moisture **Transport in Solids** 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 mts.

### DOMAIN SELECTION

If any part of the model geometry should not partake in the moisture transport, 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.

## CROSS-SECTIONAL AREA

For 1D components, enter a cross-sectional area  $A_c$  (SI unit:  $m^2$ ) to define a parameter for the area of the geometry perpendicular to the 1D component. The default value is  $1 \text{ m}^2$ .

### PHYSICAL MODEL

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

### **GRAVITY EFFECTS**

By default there are no gravity effects added. Select the check box **Include gravity** to account for the acceleration of gravity in the liquid velocity. 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.

## DEPENDENT VARIABLES

The default variable names use the pattern <name>.hr and <name>.pm for the relative humidity and moist air pressure variables.

## DISCRETIZATION

In the Moisture Transport in Solids interface, you can choose the order of the discretization for the dependent variables. The default is to use Quadratic shape functions.

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.

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



You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Domain and Boundary Nodes for the Moisture Transport in Solids Interface

The Moisture Transport in Solids Interface has these domain, boundary, and pair nodes, which are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



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

### LINKS TO FEATURE NODE INFORMATION

These nodes (and subnodes) are described in this section:

- · Porous Medium
- Liquid Water (Porous Medium)
- Moist Air (Porous Medium)
- Porous Matrix (Porous Medium)
- Initial Values

- Moisture Source
- Moisture Flux
- Moisture Content and Pressure
- No Flux
- Symmetry



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 defines the properties of a porous medium filled with two phases in equilibrium: liquid water and moist air.

Isothermal drying of porous media is driven by the difference in relative humidity in the porous medium and its surroundings. This difference in relative humidity results in the evaporation of water and the release of moisture to the environment. There exist two drying mechanisms; evacuation of moisture by vapor molecular diffusion, and evaporation of the liquid water at the surface by capillary pressure gradients in the porous solid.

The **Porous Medium** node contains three default subnodes — the Liquid Water (Porous Medium) node, the Moist Air (Porous Medium) node, and the Porous Matrix (Porous Medium) node.

## 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 settings in the **Permeability** in the Porous Matrix (Porous Medium) subnode are set according to the coordinate system selected in this section.

### MOISTURE TRANSPORT PROPERTIES

The **Moisture function** characterizes the relationship between the amount of accumulated water and the relative humidity in the porous material. The available options for the Moisture function are Moisture storage function or Capillary pressure. The selection determines how the liquid water saturation is computed.

When Moisture storage function is selected from the Moisture function list, the default Moisture storage function  $w_c(\phi_w)$  is taken From material. For User defined, enter another value or expression.

Select the **Capillary model** for the capillary flux:

- When Capillary model is set to Kelvin's law (default), a Darcy's law based on the capillary pressure is used, and the capillary pressure itself is derived from the relative humidity by using Kelvin's law, using the assumption that the liquid and gas phases are in equilibrium in the porous medium.
- When Capillary model is set to Diffusion model, the capillary flux is derived from the gradient of the moisture content and the **Moisture diffusivity**  $D_{\rm w}$ .
- For User defined, set a value for the Capillary liquid flux density,  $\Gamma_c$ , to characterize the liquid transport as a function of the moisture content.

When or Capillary pressure is selected from the Moisture function list, select the Capillary pressure model — van Genuchten or Brooks and Corey.

- For van Genuchten, enter an Entry capillary pressure  $p_{ec}$  (SI unit: Pa), the Constitutive relations constant  $m_{
  m vg}$ , the Constitutive relations constant  $l_{
  m vg}$  (dimensionless), the Liquid water residual saturation  $s_{rl}$ , and the Moist air residual saturation  $s_{rm}$ .
- For Brooks and Corey, enter an Entry capillary pressure  $p_{ec}$  (SI unit: Pa) and the Pore size distribution index  $\lambda_{
  m p}$ , the Liquid water residual saturation  $s_{
  m rl}$ , and the Moist air residual saturation  $s_{rm}$ .



See Porous Material in the COMSOL Multiphysics Reference Manual.

Q	The moist air properties are specified in the Moist Air (Porous Medium) subnode.
	The properties for liquid water convective transport are specified in the Liquid Water (Porous Medium) subnode.
	The porosity and permeability are specified in the Porous Matrix (Porous
	Medium) subnode.
<b>Q</b>	The Moisture Transport in Porous Media Interface
	Theory for Moisture Transport in Porous Media
@	For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/

## LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>Porous Medium

Ribbon

Physics tab with Moisture Transport in Solids selected:

## Domains>Porous Medium

# Liquid Water (Porous Medium)

This subnode defines the properties for the transport of water in a porous medium filled with two phases in equilibrium: liquid water and moist air.

## LIQUID WATER PROPERTIES

This section contains the settings for the definition of convective transport of liquid water. See Porous Medium for the definition of capillary transport.

The mass flux of liquid water is computed with Darcy's law. Set the Relative liquid water **permeability**,  $\kappa_{rl}$  (dimensionless), that multiplies the permeability in the Darcy's law to account for the saturation of the liquid phase.

### LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>Porous Medium>Liquid Water

Moist Air (Porous Medium)

This subnode defines the properties for the transport of the moist air phase in a porous medium filled with two phases in equilibrium: liquid water and moist air.

## MOIST AIR PROPERTIES

This section contains settings for the definition of convective and diffusive vapor transport.

The mass flux of vapor is computed with Darcy's law. Set the Relative moist air **permeability**,  $\kappa_{rm}$  (dimensionless), that multiplies the permeability in the Darcy's law to account for the saturation of the moist air phase.

Set the **Vapor diffusion coefficient**  $D_{v}$  (SI unit:  $m^{2}/s$ ) for the diffusion of vapor in air. The default value  $2.6 \cdot 10^{-5}$  m<sup>2</sup>/s is valid at T = 298 K and  $p_{mA} = 1$  atm. You may set a temperature or pressure-dependent diffusion coefficient through the use of the variables mts.T and mts.pmA.

Specify the Effective diffusivity model used to account for the porosity and the tortuosity in the effective diffusion coefficient,  $D_{\rm eff}$  (SI unit:  ${\rm m}^2/{\rm s}$ ). The available options are Millington and Quirk model (the default), Bruggeman model, Tortuosity model, and No correction.

For the **Tortuosity model** option, enter a value for the **Tortuosity factor**  $\tau$ (dimensionless). The default is 1.

## LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>Porous Medium>Moist Air

Porous Matrix (Porous Medium)

This subnode defines the properties of a porous medium filled with two phases in equilibrium: liquid water and moist air.

### POROUS MATRIX PROPERTIES

The Porosity,  $\varepsilon_{\rm p}$  (dimensionless), by default uses values From material. For User defined the default is 0.8.

Set the **Permeability**,  $\kappa$  (SI unit:  $m^2$ ), to specify the capacity of the porous material to transmit flow. The default uses values From material. For User defined select Isotropic, Diagonal, or Symmetric to enter values or expressions in the edit fields.

When a Porous Material node is defined on the domains where the Porous Medium feature is active, the Porosity and the Permeability can be set in the Homogenized **Properties** section of the **Porous Material** node.

> When setting temperature or pressure-dependent properties, the corresponding model inputs can be specified in the Porous Medium parent node.

2

The capillary transport and storage properties of the porous material can be specified in the Porous Medium parent node.

The properties for liquid transport are specified in the Liquid Water (Porous Medium) subnode.

The moist air properties are specified in the Moist Air (Porous Medium) subnode.

### LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>Porous Medium>Porous Matrix

## Initial Values

The **Initial Values** node specifies the initial values for the dependent variables. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

## INITIAL VALUES

Enter a value or expression for the initial value of the relative humidity and moist air pressure variables.

### LOCATION IN USER INTERFACE

Context Menus

# Moisture Transport in Solids>Initial Values

Ribbon

Physics tab with **Moisture Transport in Solids** selected:

### Domains>Initial Values

## Moisture Source

This node describes moisture generation within the domain. Add or remove moisture content with a positive or negative value, respectively. Add one or more nodes as needed — all moisture sources within a domain contribute with each other.

## MOISTURE SOURCE

The **Moisture Source** node adds a source term  $G_0$  to the right-hand side of the moisture transport equation.

## LOCATION IN USER INTERFACE

Context Menus

## Moisture Transport in Solids>Moisture Source

Physics tab with **Moisture Transport in Solids** selected:

### **Domains>Moisture Source**

# Moisture Flux

Use this node to add moisture flux across exterior boundaries. A positive moisture flux adds moisture to the domain. Also the external moist air pressure is prescribed.

## MOISTURE FLUX

Select the Flux type from the list: General moisture flux (the default), Convective moisture flux, concentration difference, or Convective moisture flux, pressure difference.

General Moisture Flux

It adds  $g_0$  to the total flux across the selected boundaries. Enter a positive value for  $g_0$ to represent a moisture flux that enters the domain.

Convective Moisture Flux, Concentration Difference

Enter a value for the Moisture transfer coefficient  $h_m$  together with the External temperature,  $T_{\text{ext}}$ , and the External relative humidity,  $\phi_{\text{w.ext}}$ , to compute the flux across the selected boundaries. For User defined, enter values or expressions. Else, select an Ambient relative humidity and an Ambient temperature defined in an Ambient Properties node under **Definitions**. The convective moisture flux is defined by

$$g_0 = M_{\mathbf{v}} h_m [c_{\mathbf{v}, \text{ ext}} - c_{\mathbf{v}}]$$

Convective Moisture Flux, Pressure Difference

Enter a value for the Moisture transfer coefficient  $\beta_{\it p}.$  In addition, two options are available to specify the external conditions:

• If Relative humidity is selected (the default), set the External relative humidity,  $\phi_{w.ext}$ , and the **External temperature**,  $T_{
m ext}$  (used for the computation of the vapor saturation pressure). For User defined, enter values or expressions. Else, select an Ambient relative humidity and an Ambient temperature defined in an Ambient Properties node under **Definitions**. Convective moisture flux is defined by

$$g_0 = \beta_p[\phi_{w, ext}p_{sat}(T_{ext}) - \phi_{w}p_{sat}(T)]$$

• If Partial vapor pressure is selected, enter an External partial vapor pressure,  $p_{v.ext}$ . Convective moisture flux is defined by

$$g_0 = \beta_p[p_{v, ext} - \phi_w p_{sat}(T)]$$

#### 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.

In the COMSOL Multiphysics Reference Manual:



- Constraint Reaction Terms
- · Weak Constraints
- Constraint Settings

## LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>Moisture Flux

Ribbon

Physics tab with **Moisture Transport in Solids** selected:

#### **Boundaries>Moisture Flux**

# Moisture Content and Pressure

Use this node to specify the relative humidity and the moist air pressure on exterior boundaries.

## 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.

In the COMSOL Multiphysics Reference Manual:



- Constraint Reaction Terms
- · Weak Constraints
- Constraint Settings

# LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>Moisture Content and Pressure

Ribbon

Physics tab with **Moisture Transport in Solids** selected:

**Boundaries>Moisture Content and Pressure** 

# No Flux

The No flux node is the default boundary condition on exterior boundaries. It should be used on boundaries across which there is no moisture flux. The condition corresponds to

$$\mathbf{N} \cdot \Gamma_i = 0$$

where  $\mathbf{N}$  denotes the outward pointing normal of the boundary in the reference configuration, and  $\Gamma_i$  corresponds to the moist air and humidity fluxes.

#### LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>No Flux

Ribbon

Physics tab with Moisture Transport in Solids selected:

Boundaries>No Flux

Symmetry

The **Symmetry** node can be used to represent boundaries where the species distribution is symmetric, that is, where there is no flux across the boundary. This boundary condition is identical to that of the No Flux node. It can be applied on exterior boundaries only.

## LOCATION IN USER INTERFACE

Context Menus

Moisture Transport in Solids>Symmetry

Ribbon

Physics tab with Moisture Transport in Solids selected:

**Boundaries>Symmetry** 

# Theory for Moisture Transport in Solids

In a porous material, moisture may be present in either vapor or liquid water, and moisture transport may occur through convection or diffusion.

Two fundamental phenomena are employed to elucidate the transport of liquid water within the pores of porous materials:

- Adsorption: the vapor is attached to the pore walls. Equilibrium vapor pressure is reached in the pores under thermodynamic conditions markedly distinct from those required in a free medium. Altering saturation conditions produces a notable shift in relative humidity, thereby rendering it a pertinent variable in the assessment of moisture content.
- Capillarity: when the porous medium is wetted by liquid water, there is a pressure difference between the liquid and gas (moist air) phases, due to the curvature of the wetting interface. The pressure difference, referred to as *capillary pressure*, becomes the driving force for further pore filling. Note that in some applications, the capillary pressure is replaced by the suction.

The predominance of either of these effects, adsorption or capillarity, depends on the amount of liquid water in the porous medium, and on the size and shape of the pores. Two moisture regions can be distinguished depending on the process and materials under study:

- Hygroscopic regime, where adsorption is the predominant effect. The equilibrium moisture content is better characterized by the relative humidity through the specification of a sorption curve. For a relative humidity below 95%, the slope of the sorption curve is small, and moisture content increases almost linearly as a function of the relative humidity. Building materials are mostly modeled under this assumption.
- Capillary water region, where capillarity is the predominant effect. Above 95% relative humidity, a very small variation of humidity induces a large variation of moisture content, and the *capillary pressure* formulation is best suited to characterize the moisture content through the specification of a retention curve (for example, the van Genuchten or Brooks and Corey retention models, see The Richards' Equation Interface for a description of these models).

In porous media, the relative humidity and capillary pressure are the state variables to describe the thermodynamic state of water. It is assumed that the two phases, gas and liquid, are in a state of local equilibrium and are interconnected through Kelvin's law.

As long as equilibrium conditions are upheld, the state variables are continuous when transitioning between two porous materials (such as at the interface between two materials with differing porosities) or between a porous medium and a free medium. Kelvin's law holds true on both sides of the interface.

Conversely, liquid saturation and moisture content depend upon the properties of the porous material and may experience discontinuities at interfaces between two media with distinct properties.

The Moisture Transport in Solids Interface is dedicated to the modeling of moisture transport in porous media. In the hygroscopic moisture regime, the total moisture content is defined by the sorption curve

$$w(\phi_w) = (s_l \rho_l + s_m \rho_w) \varepsilon_p$$

where the liquid saturation,  $s_1$ , describes the amount of liquid water within the pores, the moist air saturation,  $s_{\rm m}$ , describes the amount of moist air within the pores, and  $\varepsilon_{\rm p}$ is the porosity.

Alternatively, in the *capillary regime*, it is possible to use a *retention curve* that establishes the relationship between the capillary pressure,  $p_c$ , as a function of the liquid water saturation  $s_1$ :

$$p_{\rm m} = p_1 + p_{\rm c}(s_1)$$

A single equation for the transport of the total moisture content is obtained by adding the equations for the mass conservation of liquid water and vapor, and assuming local equilibrium between the liquid and gas phases. Thereafter, the evaporation and condensation source terms cancel out, and the equation of moisture transport reads

$$s_{\rm m} \rho_{\rm v} S_{\rm p}^{\rm v} p_{\rm v, \, sat} \frac{\partial \phi_{\rm w}}{\partial t} + \nabla \cdot \Gamma_{\rm w} = \varepsilon_{\rm p} (\rho_{\rm v} - \rho_{\rm l}) \frac{\partial s_{\rm l}}{\partial t} + G \tag{5-22}$$

The interface also solves for the transport of dry air to account for changes in the moist air pressure:

$$s_{\rm m} \rho_{\rm a} S_{\rm p}^{\rm a} \frac{\partial p_{\rm a}}{\partial t} + \nabla \cdot \Gamma_{\rm a} = \varepsilon_{\rm p} \rho_{\rm a} \frac{\partial s_{\rm l}}{\partial t}$$

where Dalton's law is used to relate the moist air pressure to the vapor and dry air pressures:

$$p_{\rm m} = p_{\rm v} + p_{\rm a}$$

The quantities involved are:

- $s_1$  (dimensionless) is the liquid water saturation.
- $w(\phi_w)$  (SI unit: kg/m<sup>3</sup>) is the total moisture content.
- $\phi_{w}$  (dimensionless) is the relative humidity.
- $\rho_v$  (SI unit: kg/m<sup>3</sup>) is the water vapor density.
- $\rho_1$  (SI unit: kg/m<sup>3</sup>) is the liquid water density, it can be a function of the temperature.
- $\rho_a$  (SI unit: kg/m<sup>3</sup>) is the dry air density.
- $S_{\rm p}^{\rm V}$  (SI unit: 1/Pa) is the storage coefficient for the water vapor.
- $S_{\rm p}^{\ a}$  (SI unit: 1/Pa) is the storage coefficient for the dry air.
- $p_{v.sat}$  (SI unit: Pa) is the vapor saturation pressure, that can be a function of the temperature only.
- $p_{\rm m}$  (SI unit: Pa) is the moist air pressure.
- $p_1$  (SI unit: Pa) is the liquid water pressure.
- $p_a$  (SI unit: Pa) is the dry air pressure.
- $\mathbf{v}_1$  (SI unit: m/s) is the liquid water velocity, defined by Darcy's law as

$$\mathbf{v}_1 = -\frac{\kappa_{\mathrm{rl}}\kappa}{\mu_{\mathrm{l}}} \nabla p_{\mathrm{l}}$$

- $\kappa_{rl}$  (dimensionless) is the relative liquid water permeability, that may be a function of the liquid saturation  $s_1$ .
- $\mu_1$  (SI unit: Pa·s) is the liquid water viscosity, that may be a function of the temperature.
- $\kappa$  (SI unit: m<sup>2</sup>) is the permeability of the porous medium.
- $\mathbf{v}_{\mathbf{v}}$  (SI unit: m/s) is the water vapor velocity defined by

$$\mathbf{v}_{v} = \mathbf{v}_{m} + \mathbf{v}_{vm}$$

•  $\mathbf{v}_{m}$  (SI unit: m/s) is the moist air velocity, defined by Darcy's law as

$$\mathbf{v}_{\mathrm{m}} = -\frac{\kappa_{\mathrm{rm}} \kappa}{\mu_{\mathrm{m}}} \nabla p_{\mathrm{m}}$$

- $\kappa_{rm}$  (dimensionless) is the relative moist air permeability, that may be a function of the liquid saturation  $s_1$ .
- $\mu_m$  (SI unit: Pa·s) is the moist air viscosity, that may be a function of the temperature.
- $\mathbf{v}_{vm}$  (SI unit: m/s) is the relative velocity of vapor in moist air.
- $\Gamma_c$  (SI unit: kg/m<sup>2</sup>·s) is the capillary flux that can be defined either from the capillary pressure gradient or by diffusion of relative humidity.
- $\Gamma_a$  (SI unit: kg/m<sup>2</sup>·s) is the dry air flux. It is defined as

$$\Gamma_{a} = \rho_{a} \mathbf{v}_{a}$$

•  $\Gamma_{\rm w}$  (SI unit: kg/m<sup>2</sup>·s) is the moisture (water content) flux. It is defined as

$$\Gamma_{\rm w} = \rho_{\rm l} \mathbf{v}_{\rm l} + \rho_{\rm v} \mathbf{v}_{\rm v} = -D_{\rm \phi} \nabla \phi_{\rm w} - D_{\rm p} \nabla p_{\rm m} - \Gamma_{\rm c}$$

•  $\mathbf{v}_{a}$  (SI unit: m/s) is the dry air velocity defined by

$$\mathbf{v}_{a} = \mathbf{v}_{m} + \mathbf{v}_{am}$$

- $\mathbf{v}_{am}$  (SI unit: m/s) is the relative velocity of dry air in moist air.
- G (SI unit: kg/(m<sup>3</sup>·s)) is a moisture source (or sink).

# 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. The following physics interfaces can be found under the **Heat Transfer** branch ( ) when adding a physics interface:

- · Heat Transfer in Solids
- · Heat Transfer in Fluids
- · Heat Transfer in Solids and Fluids
- Conjugate Heat Transfer, Laminar Flow
- Electromagnetic Heating, Joule Heating and Induction Heating
- Thin Structures, Heat Transfer in Fractures
- Heat and Moisture Transport:

**Building Materials** 

Moist Air

Heat and Moisture Flow, Laminar Flow

- Heat Transport in Porous Media
- Local Thermal Nonequilibrium

Some of these interfaces are available with COMSOL Multiphysics and described in the Comsol Multiphysics Reference Manual. Others are only available for the Porous Media Flow module and the Heat Transfer module. Please take a look at the Specification chart for a detailed overview of the functionality available in each product (https://www.comsol.com/products/specifications/).

In this chapter you will find assistance in selecting the right heat transfer interface for your application by getting a short overview over the different interfaces available. Furthermore, the important mechanisms of heat transfer are introduced. However, a detailed list of available domain and boundary conditions and other features for each interface as well as introductions to the theory of the implemented features are presented in the Heat Transfer Module User's Guide. You will find the links to the appropriate chapters in the text below.

Some of the physics interfaces found under the Heat Transfer branch are predefined multiphysics interfaces and are therefore described in Chapter Multiphysics Interfaces and Couplings.

# In this chapter:

- Selecting the Right Heat Transfer Interface
- The Mechanisms for Heat Transfer

# Selecting the Right Heat Transfer Interface

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. At the end of this section you will find links to the specific sections which are relevant for simulations of heat transfer in porous media.

The Heat Transfer branch included with the Porous Media Flow Module license includes a number of subbranches to describe energy transport.

The Heat Transfer in Solids Interface provides tools for analyzing heat transfer that is proportional to a temperature gradient, or conduction. The temperature equation defined in solid domains corresponds to the differential form of the Fourier's law. 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 Heat Transfer in Fluids Interface is used to model heat transfer by conduction, convection, and radiation. The temperature equation defined in fluid domains corresponds to the convection-diffusion equation that may contain additional contributions like heat sources.

A combination of both is provided in the interface The Heat Transfer in Solids and Fluids Interface and is used to model heat transfer in solids and fluids by conduction, convection, and radiation. A Solid model is active by default on all domains, and a Fluid model is also added but not active. This interface is automatically added if the precoupled multiphysics node Conjugate Heat Transfer is chosen. In this case, the Heat Transfer interface is coupled with a Laminar Flow interface. This is further described in Section The Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces.

The settings for Heat Transfer in Solids and Fluids are the same as for The Heat Transfer in Fluids Interface.

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. However, there are some enhanced features like special boundary conditions which are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

To get an overview over the functions available with the Porous Media Flow Module the following tables list the available domain and boundary conditions:

In the table below there is a list of domain nodes available in The Heat Transfer in Fluids Interface if the Porous Media Flow Module is licensed:

Fluid

• Heat Source

• Initial Values

• Moist Air (Heat Transfer Interface)

• Phase Change Material

Solid

Thickness

• Translational Motion

The Heat Transfer in Fluids Interface has the following boundary nodes available with the Porous Media Flow module:

• Boundary Heat Source

• External Temperature (Thin Layer, Thin Film, Fracture)

• Heat Flux

• Heat Source (Thin Layer, Thin Film, Fracture)

• Inflow

• Open Boundary

Outflow

 Periodic Condition (Heat Transfer Interface)

• Surface-to-Ambient Radiation (Heat Transfer Interface)

• Symmetry (Heat Transfer Interface)

• Temperature

· Thermal Insulation

• Thin Layer (Heat Transfer Interface) and Solid (Heat Transfer in Shells Interface)

The Heat Transfer in Fluids Interface has the following edge nodes (3D components only):

• Line Heat Source

The Heat Transfer in Fluids Interface has the following point nodes:

## • Point Heat Source

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. This interface therefore offers to choose specific media like a Porous Medium in general or a Building Material via the domain nodes.

To model heat transfer by conduction and convection in thin porous structures, like fractures or cracks, The Heat Transfer in Fractures Interface is available.

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 Nonisothermal Flow and Conjugate Heat Transfer Interfaces
- The Heat Transfer in Solids Interface
- The Heat Transfer in Fluids Interface
- The Heat Transfer in Porous Media Interface
- The Local Thermal Nonequilibrium Interface
- 2
- The Heat Transfer in Fractures Interface
- Theory for the Heat Transfer Module
- Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces
- Theory for Heat Transfer in Porous Media
- Theory for Heat Transfer in Thin Structures
- Theory for the Inflow Boundary Condition

A variety of modeling techniques are discussed in the following sections of the *Heat* Transfer Module User's Guide:

- Heat Transfer Variables
- Using the Boundary Conditions for the Heat Transfer Interfaces
- Handling Frames in Heat Transfer
- 2
- Heat Transfer Consistent and Inconsistent Stabilization Methods
- Heat Transfer and Fluid Flow Coupling
- Solver Settings
- See also The Heat Transfer Module Interfaces and Theory for the Heat Transfer Module

# The Mechanisms for Heat Transfer

This section includes these topics:

- · Heat Transfer in Porous Media
- Phase Change

# Heat Transfer in Porous Media

Heat transfer in porous media comes in two flavors. 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. If the heat exchange between fluid and matrix occurs practically instantly — on the time scale considered; that is, both temperatures can be assumed to be identical. Thus there is a thermal equilibrium, and the temperature equation defined in porous media domains corresponds to the convection-diffusion equation with thermodynamic properties averaging models to account for both solid matrix and fluid properties. The Heat Transfer in Porous Media Interface provides tools and support for defining an appropriate matrix model.



Performance of a Porous Microchannel Heat Sink: Application Library path

Porous\_Media\_Flow\_Module/Heat\_Transfer/porous\_microchannel\_heat\_sink

If the above assumptions cannot be made, meaning that fluid and matrix are not in thermal equilibrium, a two-temperature model is required to simulate heat transfer. The Local Thermal Nonequilibrium Interface provides tools and support for modeling the heat transfer in the solid matrix and the fluid, and the heat exchange between both phases.



Packed Bed Latent Heat Storage: Application Library path Porous\_Media\_Flow\_Module/Heat\_Transfer/packed\_bed\_latent\_heat\_storage

# 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 Celsius, 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

Porous\_Media\_Flow\_Module/Heat\_Transfer/frozen\_inclusion

# Multiphysics Interfaces and Couplings

The Porous Media Flow Module contains several predefined multiphysics interfaces to couple flow in porous media with heat transfer, species and moisture transport, solid mechanics as well as phase transport. When a predefined multiphysics interface is added from the <code>Model Wizard</code> or <code>Add Physics</code> window, it adds the constituent interfaces and the <code>Multiphysics</code> node which automatically includes one or more multiphysics couplings.

# In this chapter:

- Theory for the Poroelasticity Interfaces
- The Poroelasticity Interfaces
- Theory for the Poroelasticity, Layered Shell Interface
- The Poroelasticity, Layered Shell Interface
- Theory for the Multiphase Flow in Porous Media Interface
- The Multiphase Flow in Porous Media Interface
- The Moisture Flow Interface
- The Heat and Moisture Transport Interfaces
- The Heat and Moisture Flow Interface

- The Reacting Flow in Porous Media Interface
- The Nonisothermal Flow, Brinkman Equations Interface
- The Two-Phase Flow, Level Set, Brinkman Equations Interface

0	The Multiphysics Branch in the COMSOL Multiphysics Reference Manual.
	Coupling features are available from the context menu (right-click the <b>Multiphysics</b> node) or from the <b>Physics</b> toolbar, <b>Multiphysics Couplings</b> menu.
	Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

# 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:

$$\sigma = \mathbf{C} : \varepsilon - \alpha_{\mathbf{R}} p_{f} \mathbf{I} \tag{7-1}$$

Here,  $\sigma$  is the Cauchy stress tensor,  $\epsilon$  is the strain tensor,  $\alpha_B$  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 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 the stress tensor  $\sigma$ , as written in Equation 7-1

$$-p_{\rm m} = {\rm trace}(\sigma)/3 = K_{\rm d} \varepsilon_{\rm vol} - \alpha_{\rm B} p_{\rm f}$$

Here, the mean pressure  $p_{\rm m}$  is positive in compression,  $K_{\rm d}$  is the bulk modulus of the drained porous matrix, and the volumetric strain  $\varepsilon_{vol}$  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,  $\alpha_{\rm B}p_{\rm f}$ , as a load. In this setting, the variables for the stress tensor  $\sigma$  and mean pressure  $p_{\rm m}$  are effective stress measures.



The mean pressure and the volumetric strain are available from the Solid Mechanics interface in the variables solid.pm and solid.evol, respectively. 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  $\zeta$  to changes in volumetric strain and pore pressure. The pore pressure is proportional to the dilation of the porous matrix and the variation in fluid content:

$$p_{\rm f} = M(\zeta - \alpha_{\rm R} \varepsilon_{\rm vol}) \tag{7-2}$$

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 the Darcy's law interface. It is defined through Equation 7-2 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

$$S_{p} = \frac{\varepsilon_{p}}{K_{f}} + \frac{\alpha_{B} - \varepsilon_{p}}{K_{s}} = \varepsilon_{p} \chi_{f} + (\alpha_{B} - \varepsilon_{p}) \chi_{s}$$
 (7-3)

where  $\varepsilon_p$  is the initial porosity,  $K_f$  the fluid bulk modulus (the inverse of the fluid compressibility  $\chi_f$ ), and  $K_s$  the solid bulk modulus (the inverse of the solid compressibility  $\chi_s$ ); 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 in 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

$$\alpha_{\rm B} = \frac{\partial p_{\rm m}}{\partial p_{\rm f}} \bigg|_{\epsilon_{\rm ir}} = 1 - \frac{K_{\rm d}}{K_{\rm s}}$$

The drained bulk modulus  $K_{
m d}$  is always smaller than the solid bulk modulus  $K_{
m s}$  (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 Biot-Willis coefficient depends on the properties of the porous matrix but not on the properties of the fluid. A soft porous matrix is represented by a Biot-Willis coefficient close to unit (since  $K_d \ll K_s$ ), while for a stiff matrix,  $\alpha_B$  is close to the porosity  $\varepsilon_{\rm p}$ , since  $K_{\rm d} \approx (1 - \varepsilon_{\rm p}) K_{\rm s}$ .

By replacing  $K_s = K_d/(1 - \alpha_B)$ , the storage coefficient  $S_p$  in Equation 7-3 is calculated in terms of the porosity  $\epsilon_{\text{p}}$ , the Biot–Willis coefficient  $\alpha_{\text{B}}$ , and the bulk moduli of the fluid  $K_f$  and the drained porous matrix  $K_d$  as

$$S_{\rm p} = \frac{\varepsilon_{\rm p}}{K_{\rm f}} + (\alpha_{\rm B} - \varepsilon_{\rm p}) \frac{(1 - \alpha_{\rm B})}{K_{\rm d}}$$
 (7-4)

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  $S_p \approx \varepsilon_p / K_f$ .

A special case of Biot's theory of poroelasticity arises if both the solid and the fluid phases are assumed incompressible. In this case, it follows that  $\chi_f = \chi_s = 0$ , the Biot-Willis coefficient  $\alpha_B = 1$ , and the storage coefficient  $S_p = 0$ . The corresponding governing equations are then identical to those derived for a biphasic porous medium with incompressible solid and fluid constituents (Ref. 3). This version of the poroelasticity coupling is available by selecting the **Biphasic** poroelasticity model, see Poroelastic Coupling Properties.

The linear momentum balance for a fully saturated porous solid in equilibrium under gravitational load reads

$$-\nabla \cdot \boldsymbol{\sigma} = -\nabla (\alpha_{\rm B} p_{\rm f}) + \rho_{\rm av} \mathbf{g} \tag{7-5}$$

where  $\sigma$  is the stress tensor computed from linear elasticity, and  $\mathbf{g}$  is the gravitational acceleration. The average density  $\rho_{\text{av}}$  is computed from

$$\rho_{av} = \rho_f \varepsilon_p + \rho_d$$

where  $\rho_f$  represents the fluid density,  $\rho_d = (1 - \epsilon_p)\rho_s$  the density of the dry porous matrix, and  $\rho_s$  the density of the solid material.



The density of the dry porous matrix,  $\rho_d$ , and the drained bulk modulus,  $K_{\rm d}$ , correspond to the user inputs for the density and bulk modulus in the Solid Mechanics interface.

The fluid-to-structure coupling enters as an additional volumetric force in the momentum equation as described in Equation 7-5, 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 7-5, 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 and biological applications since the time scale of the inertial 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 7-5 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  $\mathbf{f}$  (for example, gravity), the momentum balance then reads

$$\rho_{\text{av}} \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \mathbf{\sigma} = -\nabla (\alpha_{\text{B}} p_{\text{f}}) + \mathbf{f}$$
 (7-6)

where **u** represents the solid displacement and  $\rho_{av}$  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 describes the flow and pore pressure fields in the poroelastic medium. The fluid equation comes from the mass conservation

$$\frac{\partial}{\partial t}(\rho_{\rm f}\varepsilon_{\rm p}) + \nabla \cdot (\rho_{\rm f}\mathbf{v}_{\rm d}) = Q_{\rm m} \tag{7-7}$$

where  $ho_f$  is the fluid density,  $ho_p$  is the porosity, and  $Q_m$  is a mass sink or source. The so-called Darcy velocity  $\mathbf{v}_{d}$  is computed from Darcy's law

$$\mathbf{v}_{\rm d} = -\frac{\kappa}{\mu} \nabla p_{\rm f}$$

where  $\kappa$  is the permeability of the porous matrix,  $\mu$  is the fluid viscosity, and  $p_f$  is the pore pressure. If gravity is included, Darcy's velocity is augmented by

$$\mathbf{v}_{\rm d} = -\frac{\kappa}{\mu} (\nabla p_{\rm f} - \rho_{\rm f} \mathbf{g})$$

where **g** is the gravitational acceleration. Note that the Darcy velocity  $\mathbf{v}_{\mathbf{d}}$  is actually the relative velocity of the fluid with respect to the pore walls weighted by the porosity,

$$\mathbf{v}_{d} = \varepsilon_{p}(\mathbf{v}_{f} - \mathbf{v}_{s})$$

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  $S_{\rm p}$  is calculated from Equation 7-4 for Biot poroelasticity and it is set to zero for biphasic poroelasticity.

For small strain poroelasticity, the mass source or sink  $Q_{
m m}$  reads

$$Q_{\rm m} = -\rho_{\rm f} \alpha_{\rm B} \frac{\partial}{\partial t} \epsilon_{\rm vol}$$

where  $\partial \varepsilon_{\text{vol}}/\partial t$  is the rate of change in volumetric strain (of the porous matrix),  $\rho_f$  is the fluid density, and  $\alpha_B$  is the Biot–Willis coefficient. You can interpret the right-hand-side term as the rate of expansion of the pore space. As  $\varepsilon_{vol}$  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 translate the mass conservation equation, Equation 7-7, into

$$\rho_{\rm f} S_{\rm p} \frac{\partial p_{\rm f}}{\partial t} + \nabla \cdot (\rho_{\rm f} \mathbf{v}_{\rm d}) = -\rho_{\rm f} \alpha_{\rm B} \frac{\partial}{\partial t} \varepsilon_{\rm vol} \tag{7-8}$$

# 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 7-6, reads

$$\rho_{\text{av}} \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot P^T = \nabla \cdot P_{\text{p}}^T + \mathbf{f}$$
 (7-9)

where the gradient  $\nabla = \partial / \partial \mathbf{X}$  corresponds to the material gradient with respect to the undeformed configuration, and P is the (effective) first Piola–Kirchhoff stress tensor. See Equation of Motion in the Structural Mechanics Theory chapter for details.

The pore pressure contribution enters as a load in Equation 7-9. The first Piola— Kirchhoff stress generated from the pore pressure reads

$$P_{\rm p} = -\alpha_{\rm B} p_{\rm f} J F^{-T} \tag{7-10}$$

where F is the deformation gradient and J is the volume change. In biphasic poroelasticity, the total stress in the mixture is often of interest. The corresponding Cauchy stress is computed as

$$\sigma_{\text{mix}} = \sigma - p_f I \tag{7-11}$$

where  $\sigma$  is the (effective) Cauchy stress computed in the Solid Mechanics interface.

Darcy's law is also written with respect to the undeformed configuration. The material Darcy velocity field reads

$$\mathbf{V}_{\rm d} = -\frac{\kappa}{\mu} \nabla p_{\rm f}$$

where  $\kappa$  is the material permeability tensor of the porous matrix,  $\mu$  is the fluid viscosity, and  $p_f$  is the pore pressure. 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)

$$\mathbf{v}_{\mathrm{d}} = \frac{1}{J} F \cdot \mathbf{V}_{\mathrm{d}}$$

The mass conservation, Equation 7-8, is then written as (Ref. 2)

$$\rho_{\rm f} S_{\rm p} \frac{\partial p_{\rm f}}{\partial t} + \frac{1}{J} \nabla \cdot (\rho_{\rm f} \mathbf{V}_{\rm d}) = -\rho_{\rm f} \alpha_{\rm B} \frac{\partial}{\partial t} \varepsilon_{\rm vol} \tag{7-12}$$

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 coefficient  $S_{\rm p}$  is now computed from the current porosity  $\epsilon_p$  and not from the initial porosity  $\epsilon_p^0$  of the undeformed porous matrix. The poroelastic storage (Equation 7-3) in a large strain context still reads

$$S_{\rm p} = \frac{\varepsilon_{\rm p}}{K_{\rm f}} + \frac{\alpha_{\rm B} - \varepsilon_{\rm p}}{K_{\rm s}} \tag{7-13}$$

with the important difference that the current porosity in the deformed matrix,  $\varepsilon_{\rm p}$ , is now derived from mass conservation of the solid. For Biot poroelasticity, the current (deformed configuration) porosity is expressed in terms of the volume change J and the pore pressure  $p_f$  as

$$\frac{\dot{\varepsilon_{\rm p}}}{(\alpha_{\rm B} - \varepsilon_{\rm p})} = \frac{\dot{J}}{J} + \frac{1}{K_{\rm s}} \dot{p}_{\rm f}$$

For biphasic poroelasticity, the current porosity has the simple closed-form expression

$$\varepsilon_{\rm p} = 1 - \frac{1 - \varepsilon_0}{J}$$

where  $\varepsilon_0$  stands for the initial (undeformed) porosity.

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 7-12 by the volume change J, so that it reads

$$J\rho_{\mathbf{f}}S_{\mathbf{p}}\frac{\partial p_{\mathbf{f}}}{\partial t} + \nabla \cdot (\rho_{\mathbf{f}}\mathbf{V}_{\mathbf{d}}) = -\rho_{\mathbf{f}}\alpha_{\mathbf{B}}\frac{\partial J}{\partial t}$$
 (7-14)

In the biphasic poroelasticity formulation, the first term on the left hand side is neglected as the storage coefficient  $S_p$  is set to zero.

# Unsaturated Poroelasticity

For unsaturated poroelasticity, the pore pressure is computed from the volume average of the liquid water and moist air pressures,  $p_1$  and  $p_m$ 

$$p_{\rm f} = s_{\rm l} p_{\rm l} + s_{\rm m} p_{\rm m}$$

here,  $s_1$  is the liquid saturation, and  $s_m = 1 - s_1$  is the moist air saturation.

The liquid water and moist air pressures are computed by solving the continuity equations for dry air and moisture content

$$s_{\rm m} \rho_{\rm a} S_{\rm p}^{\rm a} \frac{\partial p_{\rm a}}{\partial t} + \nabla \cdot \Gamma_{\rm a} = \varepsilon_{\rm p} \rho_{\rm a} \frac{\partial s_{\rm l}}{\partial t} - s_{\rm m} \rho_{\rm a} \alpha_{\rm B} \frac{\partial \varepsilon_{\rm vol}}{\partial t} - s_{\rm m} \rho_{\rm a} S_{\rm p}^{\rm s} \frac{\partial p_{\rm f}}{\partial t}$$

$$s_{\rm m} \rho_{\rm v} S_{\rm p}^{\rm v} p_{\rm v,\,sat} \frac{\partial \phi_{\rm w}}{\partial t} + \nabla \cdot \Gamma_{\rm w} = \varepsilon_{\rm p} (\rho_{\rm v} - \rho_{\rm l}) \frac{\partial s_{\rm l}}{\partial t} - \rho_{\rm w} \alpha_{\rm B} \frac{\partial \varepsilon_{\rm vol}}{\partial t} - \rho_{\rm w} S_{\rm p} \frac{\partial p_{\rm f}}{\partial t}$$

here,  $\rho_a$  stands for the dry air density,  $\rho_v$  is the vapor density,  $\rho_l$  is the liquid water density,  $\rho_w$  is the volume average water density (vapor and liquid), and  $\phi_w$  is the relative humidity.

The storage coefficients,  $S_{p}^{i}$  , for vapor, dry air, and solid are defined as

$$S_{\rm p}^{\rm v} = \varepsilon_{\rm p} \chi_{\rm v}$$

$$S_{\rm p}^{\rm a} = \varepsilon_{\rm p} \chi_{\rm a}$$

$$S_{\rm p}^{\rm s} = (\alpha_{\rm B} - \varepsilon_{\rm p}) \chi_{\rm s}$$

where  $\chi_i$  stands for the compressibility of the *i*-component.

For a formulation equivalent to Large Strain Poroelasticity, the continuity equations read

$$Js_{\rm m}\rho_{\rm v}S_{\rm p}^{\rm v}p_{\rm v,\,sat}\frac{\partial\phi_{\rm w}}{\partial t}+\nabla\cdot\Gamma_{\rm w}=J\epsilon_{\rm p}(\rho_{\rm v}-\rho_{\rm l})\frac{\partial s_{\rm l}}{\partial t}-\rho_{\rm w}\alpha_{\rm B}\frac{\partial J}{\partial t}-J\rho_{\rm w}S_{\rm p}^{\rm s}\frac{\partial p_{\rm f}}{\partial t}$$

$$J s_{\rm m} \rho_{\rm a} S_{\rm p}^{\rm a} \frac{\partial p}{\partial t}^{\rm a} + \nabla \cdot \Gamma_{\rm a} = J \varepsilon_{\rm p} \rho_{\rm a} \frac{\partial s_{\rm l}}{\partial t} - s_{\rm m} \rho_{\rm a} \alpha_{\rm B} \frac{\partial J}{\partial t} - J s_{\rm m} \rho_{\rm a} S_{\rm p}^{\rm s} \frac{\partial p_{\rm f}}{\partial t}$$

The moisture flux  $\Gamma_w$  and the dry air flux the  $\Gamma_a$  are described in details in the Theory for Moisture Transport in Solids chapter.

# References for the Poroelasticity Interfaces

- 1. M.A. Biot, "Mechanics of Deformation and Acoustic Propagation in Porous Media," J. Appl. Phys., vol. 33, pp. 1482-1498, 1962.
- 2. O. Coussy, Poromechanics, John Wiley & Sons, 2004.
- 3. W. Ehlers, "Foundations of multiphasic and porous materials," Porous Media: Theory, Experiments and Numerical Applications, W. Ehlers and J. Bluhm, eds., Springer-Verlag, 2002

# The Poroelasticity Interfaces

# The Poroelasticity, Solid Interface

The **Poroelasticity, Solid** interface ( ) 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, the 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 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 the 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 7-1: 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 <b>Poroelastic storage</b> model is added by default.
Poroelasticity	The <b>Domain Selection</b> 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/Poromechanics/multilateral\_well

# Poroelasticity (Multiphysics Coupling)

The **Poroelasticity** multiphysics coupling node ( ) links the Solid Mechanics and Darcy's Law interfaces bidirectionally 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.

## **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 if 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.

#### POROELASTIC COUPLING PROPERTIES

In the Poroelasticity model list, choose between Biot and Biphasic. The Biot poroelasticity model (default) is commonly used in geotechnical applications where the compressibility of the solid and/or fluid phase is important. In contrast, the biphasic model assumes that both the solid and the fluid phases are incompressible, which is valid for soft materials like biological tissues and hydrogels. Note that even if both constituents are modeled as incompressible, the porous medium can still undergo large volume changes as a result of fluid inflow or outflow.

In the Reference pressure level list, choose User defined to 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. If applicable, the list also contains options to inherit the value from another physics interface that announces the reference pressure level as a model input. For example, the reference pressure level can often be inherited from the corresponding input in the Darcy's Law interface that is part of the Poroelasticity coupling.

For the **Biot-Willis coefficient** list, the default is to take its value **From material**. Choose **User defined** to enter a Biot–Willis coefficient  $\alpha_B$  (dimensionless) in the text field. The user input is only required if the Poroelasticity model is set to Biot.

# Theory for the Poroelasticity, Layered Shell Interface

The Theory for the Poroelasticity, Layered Shell interface is basically the same as described in Theory for the Poroelasticity Interfaces. The main difference is the 2D approximation for layered materials. Theoretical background about the 2D approximation is given in the theory chapters of the two coupled interfaces Layered Shell and Layered Darcy's Law.

All relevant information can be found in the following chapters:

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- Theory for the Poroelasticity Interfaces.
- Theory for the Layered Darcy's Law Interface.
- Theory for the Layered Shell Interface in the Structural Mechanics Module User's Guide.

# The Poroelasticity, Layered Shell Interface

The **Poroelasticity, Layered Shell** interface ( ) combines the **Layered Darcy's Law** formulation with the **Layered Shell** interface for structural mechanics. This multiphysics interface is only available for 3D simulations and is only active on all boundaries where a layered material is defined.

A layered material can be defined on the boundaries by adding one of the following nodes:

• Single Layer Material

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- Layered Material Link, together with a Layered Material node
- Layered Material Stack, together with one or several Layered Material nodes
- Material, with the Layer thickness property specified

See Layered Material, Layered Material Link, Layered Material Stack, Layered Material Link (Subnode), and Single Layer Materials in the COMSOL Multiphysics Reference Manual for details on the definition of layered materials.

This multiphysics interface is only available when the Structural Mechanics Module, the Composite Materials Module and the Porous Media Flow Module are licensed. For a detailed overview of the functionality available in each product visit <a href="https://www.comsol.com/products/specifications/">https://www.comsol.com/products/specifications/</a>.

The coupling occurs on the boundary level, where the pore pressure from the Layered Darcy's Law interface acts as a load for the Layered Shell 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, Layered Shell** interface is added from the **Structural Mechanics** branch ( ) of the **Model Wizard** or **Add Physics** windows, **Layered Shell** and **Layered Darcy's Law** interfaces are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the Poroelasticity, Layered multiphysics coupling.

For the settings of each of the coupled interfaces see



- The Layered Darcy's Law Interface and
- The Layered Shell Interface in the Structural Mechanics Module User's Guide.

## SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, as in this case Poroelasticity, Layered Shell, 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 Layered Shell and Layered 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 7-2: MODIFIED SETTINGS FOR A POROELASTICITY INTERFACE.

PHYSICS INTERFACE OR COUPLING FEATURE	MODIFIED SETTINGS
Layered Shell	For the Layered Shell interface, under Structural Transient Behavior the Structural transient behavior is set to Quasistatic.
Layered Darcy's Law	For the Layered Darcy's Law interface, under Discretization, the shape function order for the temperature is set to <b>Linear</b> . Also, a <b>Poroelastic Storage</b> model is added by default.
Poroelasticity, Layered	The corresponding Layered Shell and Layered Darcy's Law interfaces are preselected in the Coupled Interfaces section.

The **Poroelasticity, Layered** multiphysics coupling node ( ) links bidirectionally the Layered Shell and Layered Darcy's Law interfaces to account for poroelastic deformation on layered shells.

#### 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** is poro, followed by the number of defined multiphysics couplings, that is poro1 for the first multiphysics coupling feature in the model.

#### **BOUNDARY SELECTION**

When Poroelasticity, Layered is added to the Multiphysics node as an effect of adding a Poroelasticity, Layered Shell interface, the selection is the same as for the participating physics interfaces. In the Boundary Selection menu you can choose between Manual and All boundaries, the latter being the default option. Note that only boundaries that are active in the physics interfaces selected in the Coupled Interfaces section can be selected.

### COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The Layered **shell** 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 Layered shell 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.

#### SHELL PROPERTIES

Here you select on which layers of a layered material the physics interface should be active. By default, the **Use all layers** check box is selected. This means that all layers in all layered materials on the selected boundaries are used.

If you clear the Use all layers check box, you can select individual layers within a single layered material. This means that the physics interface is restricted to the boundaries on which a specific layered material is defined.



For a general description of layer selections, see The Shell Properties and Interface Selection Sections in the Structural Mechanics Module User's Guide.

## 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  $\alpha_B$  (dimensionless) in the text field.

## Theory for the Multiphase Flow in Porous Media Interface

The model equations that are solved in the Multiphase Flow in Porous Media interface are based on the mass conservation of each phase and on an extended Darcy's law. The mass conservation equation for each phase is given by

$$\frac{\partial}{\partial t} (\varepsilon_{p} \rho_{i} s_{i}) + \nabla \cdot (\rho_{i} \mathbf{u}_{i}) = Q_{i}$$
 (7-15)

where  $\varepsilon_{p}$  (dimensionless) is the porosity, and the vector  $\mathbf{u}_{i}$  should be interpreted as the volumetric flux of phase i (SI unit  $m^3/(m^2 \cdot s)$  or m/s). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_{i} = -\frac{\kappa_{\mathrm{r}i}}{\mu_{i}} \kappa(\nabla p_{i} - \rho_{i}\mathbf{g})$$
 (7-16)

where  $\kappa$  denotes the permeability (SI unit: m<sup>2</sup>) of the porous medium, **g** the gravitational acceleration vector (SI unit:  $m/s^2$ ), and  $\mu_i$  the dynamic viscosity (SI unit: kg/(m·s)),  $p_i$  the pressure field (SI unit: Pa), and  $\kappa_{ri}$  the relative permeability (dimensionless) of phase i, respectively. The phase pressures  $p_i$  are related through the capillary pressure functions  $p_{c_0}$ :

$$p_i - p_j = p_{c_{ij}}(s_1, ..., s_N) \qquad i \neq j$$
 (7-17)

One phase pressure can be chosen independently so that N-1 capillary pressure relations are needed to define the other phase pressures. In addition it is assumed that all phases together fill the pore space completely, so that we have

$$\sum_{i=1}^{N} s_i = 1 \tag{7-18}$$

### Pressure-Saturation Formulation

The algebraic relations in Equation 7-17 and Equation 7-18 allow for a reduction of the number of dependent variables. An often used way is to eliminate N-1 phase pressures and one of the saturations. This results in a so-called pressure-saturation

formulation (Ref. 3). The procedure in the Multiphase Flow in Porous Media interface is to pick one of the phases, let us say phase  $i_c$ , then express the volume fraction, or saturation,  $s_i$ , of this phase in terms of the saturations of the other phases and in addition to use the pressure,  $p_{i_e}$ , of this phase to define the other phase pressures:

$$s_{i_{c}} = 1 - \left(\sum_{i=1, i \neq i_{c}}^{N} s_{i}\right)$$
 (7-19)

$$p_i = p_{i_c} + p_{c_i}(s_1, ..., s_N)$$
 for  $i \neq i_c$  (7-20)

The equations for the saturations  $s_i$ ,  $(i \neq i_c)$  are given by Equation 7-15 and Equation 7-16. To arrive at an equation for  $p_i$ , the conservation equations of all phases are summed. This results in

$$\frac{\partial}{\partial t} \left( \varepsilon_{p} \sum_{i=1}^{N} \rho_{i} s_{i} \right) + \nabla \cdot \left( \sum_{i=1}^{N} \rho_{i} \mathbf{u}_{i} \right) = Q_{\text{tot}}$$
 (7-21)

where the total mass source  $Q_{
m tot}$  is given by

$$Q_{\text{tot}} = \sum_{i=1}^{N} Q_i \tag{7-22}$$

The equations for the saturations  $s_i$  are solved in the **Phase Transport in Porous Media** interface (Equation 7-15 and Equation 7-16). The Equation 7-21 for the pressure field  $p_{i}$ , 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

$$\frac{\partial}{\partial t} (\varepsilon_{\rm p} \rho_{\rm tot}) + \nabla \cdot (\rho_{\rm tot} \mathbf{u}_{\rm d}) = Q_{\rm m} \quad \text{where} \quad \mathbf{u}_{\rm d} = -\frac{1}{\mu} \kappa (\nabla p - \rho_{\rm tot} \mathbf{g}) \tag{7-23}$$

which is originally implemented in the **Darcy's Law** interface, with Equation 7-21 by adding the following terms to the left-hand side of Equation 7-23:

$$\nabla \cdot \left( \sum_{i=1}^{N} \rho_{i} \mathbf{u}_{i} - \rho_{\text{tot}} \mathbf{u}_{d} \right)$$
 (7-24)

and by setting the right-hand side  $Q_{\rm m}$  to be equal to  $Q_{\rm tot}$ . The volume averaged density  $\rho_{tot}$  is given by

$$\rho_{\text{tot}} = \sum_{i=1}^{N} \rho_i s_i \tag{7-25}$$

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<sup>-6</sup> m<sup>2</sup>s<sup>-1</sup> (kinematic viscosity of water at 293.15 K).

In the other direction, the multiphysics coupling node provides the averaged density (denoted by  $\rho_{tot}$  in Equation 7-24 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

$$Q_{i_c} = -\sum_{i=1, i \neq i_c}^{N} Q_i \tag{7-26}$$

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  $Q_{\mathrm{tot}}$  is supplied as a right-hand side to the Darcy Equation 7-21 for  $p_{i_a}$ .

### 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,  $p_i$ . If the pressure of another phase needs to supplied, then take into account the capillary pressure.

Since the coupled Darcy's Law interface uses the conservation equation for the total mass (Equation 7-21) to solve for  $p_i$ , the Mass Flux boundary condition in the Darcy's **Law** interface should be used to prescribe the mass flux of all phases together.

If the mass flux of the phase computed from the volume constraint needs to be prescribed at a boundary, and the total mass flux is not known a priori, it might be necessary to compute for the total mass flux in the form of a Lagrange multiplier by using the weak constraint formulation for the pressure boundary condition in the Darcy's Law interface.

### Thin Barrier (Multiphysics Coupling)

The Thin Barrier multiphysics coupling uses the Extra Dimension tool to solve the equations for the pressure and saturations through the thin barrier structure's thickness. The thin structure has its domain represented by the product space between the lumped boundary and the additional dimension for the thickness. Inside this product space, it is convenient to split the gradient operator into a tangential part and a normal part:  $\nabla = \nabla_t + \nabla_n$ .

The following assumptions, used in deriving the Thin Barrier equations from the equations solved in the Multiphase Flow in Porous Media interface, justify the simplification  $\nabla = \nabla_{\mathbf{n}}$ :

- A thin barrier can be considered as a boundary of thickness significantly smaller than the typical lengths of the overall model.
- The permeability of the porous material inside the thin barrier is significantly smaller than the permeability of the porous material in the adjacent domains.
- There is no mass source or sink inside the thin barrier.

In addition, these assumptions imply that the effect of gravity on the phase transport can be neglected. This results in the following set of equations for the saturations  $s_i$ ,  $(i \neq i_c)$  and the pressure  $p_{i_c}$ :

$$\frac{\partial}{\partial t} (\varepsilon_{\mathbf{p}} \rho_i s_i) + \nabla_{\mathbf{n}} \cdot (\rho_i \mathbf{u}_i) = 0 \quad \text{for} \quad i \neq i_c$$
 (7-27)

$$\mathbf{u}_{i} = -\frac{\kappa_{\mathrm{r}i}}{\mu_{i}} \kappa \nabla_{\mathbf{n}} p_{i} \tag{7-28}$$

$$\frac{\partial}{\partial t} \left( \varepsilon_{p} \sum_{i=1}^{N} \rho_{i} s_{i} \right) + \nabla_{\mathbf{n}} \cdot \left( \sum_{i=1}^{N} \rho_{i} \mathbf{u}_{i} \right) = 0$$
 (7-29)

Together with the algebraic relations

$$s_{i_{c}} = 1 - \left(\sum_{i=1, i \neq i_{c}}^{N} s_{i}\right)$$
 (7-30)

$$p_i = p_{i_c} + p_{c_i}(s_1, ..., s_N)$$
 for  $i \neq i_c$  (7-31)

Here  $\varepsilon_p$  (dimensionless) denotes the porosity and  $\kappa$  the permeability (SI unit: m<sup>2</sup>) of the porous material in the thin barrier. Further more  $\rho_i$  denotes the density (SI unit: kg/m<sup>3</sup>),  $\mu_i$  the dynamic viscosity (SI unit: kg/(m·s)),  $p_i$  the pressure field (SI unit: Pa),  $\mathbf{u}_i$  the (normal) volumetric flux (SI unit: m/s) and  $\kappa_{ri}$  the relative permeability (dimensionless) of phase i, respectively.

Since the interfaces between the thin barrier and the adjacent domains are boundaries between a more permeable and a less permeable porous domain, conditions analogous to the Porous Medium Discontinuity Boundary Condition are needed to couple the equation Equation 7-27 for the saturations inside the thin barrier to the equations in the adjacent domains. These condition at the extremities of the extra dimension can be written as:

$$p_{c_{i}}^{t}(s_{i}^{t})_{L=0} = \begin{cases} p_{\text{ec}, i}^{t} & \text{if} & p_{c_{i}}^{d}(s_{i}^{d}) \leq p_{\text{ec}, i}^{t} \\ p_{c_{i}}^{d}(s_{i}^{d}) & \text{if} & p_{c_{i}}^{d}(s_{i}^{d}) > p_{\text{ec}, i}^{t} \end{cases}$$
 for  $i \neq i_{c}$  (7-32)

where the superscript t is used to indicate the saturation and capillary pressure inside the thin barrier (the low permeable side of the interface), and the superscript d indicates the domain adjacent to the downside of the thin barrier (the high permeable side), and

$$p_{c_{i}}^{t}(s_{i}^{t})_{L=d_{s}} = \begin{cases} p_{\text{ec}, i}^{t} & \text{if} & p_{c_{i}}^{u}(s_{i}^{u}) \leq p_{\text{ec}, i}^{t} \\ p_{c_{i}}^{u}(s_{i}^{u}) & \text{if} & p_{c_{i}}^{u}(s_{i}^{u}) > p_{\text{ec}, i}^{t} \end{cases}$$
 for  $i \neq i_{c}$  (7-33)

where the superscript u indicates the domain adjacent to the upside of the thin barrier (again the high permeable side) and where  $d_s$  is the length of the extra dimension, or equivalently, the thickness of the thin structure.

The additional conditions are continuity of the fluxes for all phases and continuity of the pressure of the phase  $i_c$  computed from the volume constraint. Note that this last condition assumes that this phase is present both inside the thin barrier and in the adjacent domains. Furthermore, this boundary condition assumes that the phase  $i_c$ computed from the volume constraint is the wetting phase and it is necessary that the settings for the van Genuchten or Brooks and Corey capillary pressure model in the adjacent domains match this assumption.

Please find related information under



- Theory for the Phase Transport Interfaces in the CFD Module User's Guide and
- Using Extra Dimensions in the COMSOL Multiphysics Reference Manual.

### References

- 1. J. Bear, Dynamics of Fluids in Porous Media, Elsevier Scientific Publishing, 1972.
- 2. Z. Chen, G. Huan, and Y. Ma, Computational Methods for Multiphase Flows in Porous Media, Philadelphia: Society for Industrial and Applied Mathematics, 2006.
- 3. R. Helmig, Multiphase Flow and Transport Processes in the Subsurface A Contribution to the Modeling of Hydrosystems, Springer-Verlag, 1997.

## The Multiphase Flow in Porous Media Interface

The Multiphase Flow in Porous Media interface ( 🌄 ) combines the Darcy's Law interface with the Phase Transport in Porous Media interface to model the flow and transport of multiple immiscible phases in a porous medium.

When a predefined Multiphase Flow in Porous Media interface is added from the Porous Media and Subsurface Flow branch ( ) of the Model Wizard or Add Physics window, Phase Transport and Darcy's Law interfaces are added to the Model Builder. In addition, the Multiphysics node is added, which automatically includes the Multiphase Flow in Porous Media multiphysics coupling.

On the Constituent Physics Interfaces

The Phase Transport in Porous Media interface is used to simulate the transport of immiscible multiple species in a porous medium and solves for their averaged volume fractions (also called saturations). The interfaces between the different phases are not tracked explicitly, although microscopic interfacial effects are taken into account in the macroscopic equations through the capillary pressure functions.

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows in media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

#### SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example Multiphase Flow in Porous Media, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single Phase Transport in Porous Media and Darcy's Law interfaces are added, an empty Multiphysics node appears in the model tree. You can choose from the available coupling features but the settings in the constituent interfaces are not modified.

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

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- 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**  $d_{\mathbf{w}}(\mathrm{SI}\ \mathrm{unit};\mathrm{m}).$ 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  ${\it Mass flux}\,N_{0,i}$ (SI unit: kg/(m<sup>2</sup>·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

$$M_{l,i} = \rho_i s_{0,i} V_l \tag{7-34}$$

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  $M_{l,i}$  is given. Then  $V_l$  can be computed from the relation

$$V_{1} = \frac{M_{1,1}}{\rho_{1}} + \sum_{i=2}^{p} V_{1} s_{i,0} + \sum_{i=p+1}^{N} \frac{M_{1,i}}{\rho_{i}}$$
 (7-35)

where the mass flow rate  $M_{1,1}$  for the phase computed from the volume constraint is given by

$$M_{l, 1} = M_{l} - \sum_{i=2}^{p} V_{l} \rho_{i} s_{i, 0} - \sum_{i=p+1}^{N} M_{l, i}$$
 (7-36)

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  $M_{l,i}$  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  $M_{l,i}$  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  $\lambda_r = \sum_{i=1}^N \frac{\rho_i \kappa_{ri}}{\mu_i}$  (7-37)

where  $\kappa_{ri}$  denotes the relative permeability of phase *i*.

### Thin Barrier (Multiphysics Coupling)

The Multiphase Flow in Porous Media ( ) interface contains an optional Thin Barrier multiphysics coupling feature on edges (in 2D) or surfaces (in 3D). The Thin Barrier coupling node can be used to avoid meshing interior permeable structures that are less permeable than the adjacent porous domains. It links bidirectionally the **Phase** Transport in Porous Media and Darcy's Law interfaces.

#### SETTINGS

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

The default Name (for the first Thin Barrier multiphysics coupling feature in the model) is thls1.

#### **BOUNDARY SELECTION**

When nodes are added from the context menu, you can select Manual (the default) from the **Selection** list to choose specific boundaries, or select **All boundaries** as needed.

#### COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the Phase transport or Flow in porous media lists

#### SHELL PROPERTIES

The **Thin Barrier** multiphysics coupling feature is designed to be only applicable for a Single Layer Material. Select the Single Layer Material to be used for the thin barrier from the Layer list. The Thickness of the thin barrier is set in the Layer Definition section of the Shell Property Group window of the Single Layer Material. Also use this section to set the number of Mesh elements that are used in the Extra Dimension to solve the equations through the thickness of the thin barrier layer.

#### MODEL INPUT

The material properties of the different phases, such as density and viscosity, can be defined through user inputs, variables, or by selecting a boundary material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties. These model inputs appear in this section.

#### MATRIX PROPERTIES

Select the material to use as porous matrix inside the thin barrier. Select Boundary material (the default) from the Porous material list to use the material defined for the thin barrier boundary. Select another material to use that material's properties.

The default **Porosity**  $\varepsilon_{\rm p}$  (a dimensionless number between 0 and 1) uses the value **From** material, defined by the Porous material selected. For User defined the default is 0.5.

The default **Permeability**  $\kappa$  (SI unit: m<sup>2</sup>) uses the value **From material**, as defined by the **Porous material** selected. For **User defined** the default is 1e-9 m<sup>2</sup>.

#### CAPILLARY PRESSURE

Select a Capillary pressure model — User defined (the default), van Genuchten, Brooks and Corey, or Capillary diffusion. The van Genuchten and Brooks and Corey options are only available when there are not more than two phases present in the model.

- For User defined, enter an expression for the Capillary pressure  $p_c$  (SI unit: Pa) for the phases that are not computed from the volume constraint. The pressure of the corresponding phase is equal to the pressure of the phase computed from the volume constraint plus the capillary pressure supplied for this phase.
- For van Genuchten, enter an Entry capillary pressure  $p_{ec}$  (SI unit: Pa), the Constitutive relations constant  $m_{\rm vG}$  (dimensionless), and Constitutive relations constant  $l_{\rm vG}$ (dimensionless).
- For Brooks and Corey, enter an Entry capillary pressure  $p_{\mathrm{ec}}$  (SI unit: Pa) and the Pore size distribution index  $\lambda_{\mathbf{p}}$  (dimensionless).
- For Capillary diffusion, enter a capillary diffusion coefficient  $D_c$  (SI unit:  $m^2/s$ ) for the phases that are not computed from the volume constraint.

#### PHASE PROPERTIES

Select the material to use for each phase. Select **Boundary material** (the default) from the Fluid list to use the material defined for the domain. Select another material to use that material's properties.

Enter the **Density**  $\rho$  (SI unit: kg/m<sup>3</sup>), **Dynamic viscosity**  $\mu$  (SI unit: Pa·s) and **Relative permeability**  $\kappa_r$  (a dimensionless number between 0 and 1) for each phase. The defaults for the Density and Dynamic viscosity are From material, and User defined for the Relative **permeability.** For **User defined**, the default values are  $1000 \text{ kg/m}^3$ , 0.001 Pa·s. and  $s_i^2$ , respectively.

The Relative permeability input fields are only available when the Capillary pressure model is set to User defined or Capillary diffusion. In the other cases (van Genuchten or **Brooks and Corey**) the relative permeabilities are defined by the van Genuchten or Brooks and Corey model. For the van Genuchten and Brooks and Corey model, specify the **Residual saturation**  $s_{ri}$  (dimensionless, default value 0) for each phase.

### INITIAL VALUES

Enter a value or expression in the field for the volume fraction inside the thin barrier of each phase, except for the one computed from the volume constraint, and in the field for the pressure of the phase computed from the volume constraint.

Please find related information under



- Single Layer Materials in the COMSOL Multiphysics Reference Manual and
- Theory for the Multiphase Flow in Porous Media Interface in the Subsurface Flow Module User's Guide.

## The Moisture Flow Interface

The Moisture Flow interfaces model moisture transport in air by vapor diffusion and convection.

When a Moisture Flow ( ) multiphysics interface is added from the Chemical Species Transport>Moisture Flow branch of the Model Wizard or Add Physics windows, the Single-Phase Flow interface Laminar Flow and a Moisture Transport in air interface are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the Moisture Flow multiphysics coupling feature.

Although the Moisture Flow interface can be found under the Chemical Species **Transport** branch, it has been implemented in the Heat Transfer Module and made available for the Porous Media Flow Module. Therefore, detailed information is available in the Heat Transfer Module User's Guide.



- The Moisture Flow Interfaces
- Theory for the Moisture Flow Interface

## The Heat and Moisture Transport Interfaces

The Heat and Moisture Transport interfaces couple heat transfer and moisture transport in building materials and moist air.

The Building Materials version of the Heat and Moisture Transport multiphysics interface combines the Heat Transfer in Building Materials and Moisture Transport in Building Materials interfaces. A Heat and Moisture multiphysics node is automatically added to couple these interfaces. It takes in account heat and moisture storage, latent heat effects, and liquid and convective transport of moisture. In addition, the temperature dependency of the moisture properties is automatically accounted for.

When the Moist Air version of the predefined Heat and Moisture Transport interface is added, it combines the Heat Transfer in Moist Air and Moisture Transport in Air interfaces to model coupled heat and moisture transport in moist air, by modeling moisture transport by vapor diffusion and convection and heat transfer by conduction and convection with moisture-dependent thermodynamics properties.

> The versions of the Heat and Moisture Transport multiphysics interface are described in the Heat Transfer Module's User's Guide:



- The Building Materials Version of the Heat and Moisture Transport Multiphysics Interface
- The Moist Air Version of the Heat and Moisture Transport Multiphysics Interface

## The Heat and Moisture Flow Interface

The Heat and Moisture Flow interface available with the Porous Media Flow Module model heat and moisture transport in air by laminar flow.

When a Heat and Moisture Flow multiphysics interface is added from the Heat Transfer>Heat and Moisture Transport>Heat and Moisture Flow branch of the Model Wizard or Add Physics windows, a Laminar Flow, a Heat Transfer in Moist Air interface, and a Moisture Transport in air interface are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the Moisture Flow, Heat and Moisture, and Nonisothermal Flow multiphysics coupling features.

> The documentation for this interface is available in the Heat Transfer Module User's Guide



- The Heat and Moisture Flow Interfaces
- Theory for the Heat and Moisture Flow Interfaces

## The Reacting Flow in Porous Media Interface

The Reacting Flow in Porous Media, Transport of Diluted Species interface ( **[88]**) 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, 2D axial symmetry, and 3D.

Detailed information is available in the Chemical Reaction Engineering User's Guide in the section The Reacting Flow in Porous Media Multiphysics Interfaces.

# The Nonisothermal Flow, Brinkman Equations Interface

The Nonisothermal Flow, Brinkman Equations multiphysics coupling 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.

By default in the Settings window for Brinkman Equations, the Compressibility option is set to Weakly compressible flow. The Density  $\rho$  in the Porous Medium>Fluid subnode is automatically set to the variable from the Nonisothermal Flow multiphysics coupling feature. Other options for Compressibility are Incompressible flow or Compressible flow (Ma<0.3).

For Heat Transfer in Porous Media in the Porous Medium>Fluid subnode, the Absolute pressure,  $p_A$  (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 settings for the interfaces and the coupling feature are described fully under the following links:

- The Nonisothermal Flow, Brinkman Equations Interface in the CFD Module User's Guide.
- The Brinkman Equations Interface
- The Heat Transfer in Porous Media Interface in the Heat Transfer Module User's Guide

For more general information on Nonisothermal Flow see

- 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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# The Two-Phase Flow, Level Set, Brinkman Equations Interface

This Multiphysics interface was designed to track the interface between two immiscible fluids within a porous medium as for example when simulating resin transfer molding.

The tracking is done using the Level Set equation, and the velocity field for this equation can be calculated from the Brinkman Equations.

The immiscible fluids can be incompressible or compressible. The interface is available in 2D, 2D axial symmetric, and 3D.

When adding the Two-Phase Flow, Level Set, Brinkman Equations multiphysics interface, a Brinkman Equations and a Level Set interface are added to the Model Builder. In addition, the multiphysics coupling feature Two-Phase Flow, Level Set is created automatically under the Multiphysics node (see The Two-Phase Flow, Level Set Coupling Feature in the CFD Module User's Guide). The Wetted Wall coupling feature is also added, but with empty selection. Other Wetted Wall multiphysics coupling features and the Interior Wetted Wall coupling feature can be added when needed to model walls. For more information about these coupling features read The Wetted Wall Coupling Feature and The Interior Wetted Wall Coupling Feature in the CFD Module User's Guide.

Simulations using the Two-Phase Flow, Level Set, Brinkman equations interface are always time-dependent since the position of an interface is almost always dependent of its history.

Note that this multiphysics coupling does not include capillary effects arising inside the porous structure itself as these effects can be neglected for relatively high flow velocities. If these effects should be taken into account, use the Multiphysics interface The Multiphase Flow in Porous Media Interface which couples Darcy's Law with a Phase transport equation including capillary pressure and relative permeabilities.

Use the following links to get more information about the Brinkman Equations and the Level Set interfaces and the coupling features.

• The Brinkman Equations Interface

- Theory for the Brinkman Equations Interface
- The Level Set Interface in the CFD Module User's Guide
- Theory for the Level Set Interface in the CFD Module User's Guide
- The Two-Phase Flow, Level Set and Phase Field Interfaces in the CFD Module User's Guide
- Theory for the Two-Phase Flow Interfaces in the CFD Module User's Guide.

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