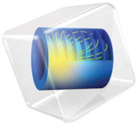

# Subsurface Flow Module

## User’s Guide

5.4

COMSOL

# Subsurface Flow Module User's Guide

Version: COMSOL 5.4

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Part number: CM020701

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## Chapter 2: Single-Phase Flow Interfaces

## Chapter 3: Porous Media and Subsurface Flow Interfaces

## Chapter 4: Chemical Species Transport Interfaces

## Chapter 5: Heat Transfer Interfaces

## Chapter 6: Structural Mechanics Interfaces

# 1

# Introduction

This guide describes the Subsurface Flow Module, an optional add-on package that extends the COMSOL Multiphysics® modeling environment with customized physics interfaces for modeling of subsurface flow.

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

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

# About the Subsurface Flow Module

This section includes these topics:

- How the Subsurface Flow Module Helps Improve Your Modeling
- Where Do I Access the Documentation and Application Libraries?

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

## *How the Subsurface Flow Module Helps Improve Your Modeling*

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

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

The physics interfaces, options, and functions are tailored to account for subsurface flow and geologic process terminology. The Heat Transfer interfaces, for example, include features to superpose a background geotherm without incorporating it as a boundary condition. These physics interfaces also include options to automate the calculation of effective thermal properties for multicomponent systems.

The Fluid Flow branch represent a wide range of possibilities. The Richards' Equation interface describes nonlinear flow in variably saturated porous media. The options for saturated porous media include the Darcy's Law interface for slow flow and the

Brinkman Equations interface where shear is non-negligible. The Laminar Flow interface uses the Navier-Stokes equations to cover free flows and the Fracture Flow interface is used for modeling flow in fractures.

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

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

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

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

### THE DOCUMENTATION AND ONLINE HELP

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

#### *Opening Topic-Based Help*

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

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Win

To open the **Help** window:

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

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Mac

Linux

To open the **Help** window:

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

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### *Opening the Documentation Window*

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Win

To open the **Documentation** window:

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

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Mac

Linux

To open the **Documentation** window:

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

### THE APPLICATION LIBRARIES WINDOW

Each model or application includes documentation with the theoretical background and step-by-step instructions to create a model or app. 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.

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

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*Opening the Application Libraries Window*

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

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Win

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

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

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Mac

Linux

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

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

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### COMSOL ACCESS AND TECHNICAL SUPPORT

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### 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/support/updates |
| COMSOL Blog | www.comsol.com/blogs |
| Discussion Forum | www.comsol.com/community |
| Events | www.comsol.com/events |
| COMSOL Video Gallery | www.comsol.com/video |
| Support Knowledge Base | www.comsol.com/support/knowledgebase |

# Modeling with the Subsurface Flow Module

This section includes these topics:

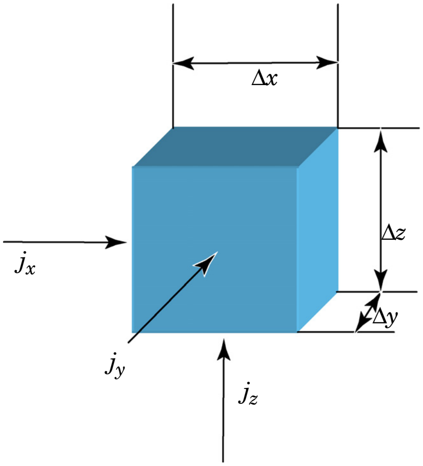
- Where Do I Start with Subsurface Flow Modeling?
- About Using the Transport of Diluted Species in Porous Media Interface
- The Subsurface Flow Module Physics Interface Guide
- Common Physics Interface and Feature Settings and Nodes
- Subsurface Flow Module Study Availability
- The Liquids and Gases Materials Database

## *Where Do I Start with Subsurface Flow Modeling?*

Many of the physics interfaces (see The Subsurface Flow Module Physics Interface Guide) have predefined equations or sets of equations adapted to earth-science applications. These are based on the equations for momentum transport (fluid flow), energy transport (heat transfer), and mass transport. You can take the equations in these physics interfaces and the variables they offer and then modify them, link them together, and couple them to physics interfaces elsewhere in COMSOL Multiphysics.

Numerical modeling typically begins with a question about some physical phenomenon within a particular region of interest. Defining the question well means that the type of information needed to answer it is obvious. Then identify which physics are actually important to answering the question and how they interact. Next a mathematical model is defined to fit to this conceptual model of the physics for the domain of interest. The mathematical model contains governing equations with boundary conditions and possibly initial conditions. The boundary conditions detail how the model domain interacts with the surrounding environment. The initial conditions make up a snapshot of the physics at some initial time. After the software solves the mathematical model, the results are interpreted in light of the original question.

In COMSOL Multiphysics you solve equation-based models of physical processes by balancing modeled entities, for example, mass or heat (energy). To balance a given modeled entity $u$, examine its flux $\mathbf{j}$ in a unit cell at a given time $t$. In this case, $u$ might represent mass or heat per unit volume where



$$\Delta x\Delta y\Delta z\frac{u_{t+\Delta t}-u_t}{\Delta t} = -\Delta y\Delta z(j_{x+\Delta x}-j_x)-\Delta x\Delta z(j_{y+\Delta y}-j_y)$$
$$-\Delta x\Delta y(j_{z+\Delta z}-j_z)+\Delta x\Delta y\Delta zF$$

In this equations the term on the left-hand side represents accumulation or the change in the amount of $u$ stored in some time period $\Delta t$. The final term on the right-hand side represents a volume source or sink. The terms in between represent the difference in the fluxes across the surfaces of the volume. Dividing both sides by $\Delta x\Delta y\Delta z$ gives the equation

$$\frac{u_t-u_{t-\Delta t}}{\Delta t} = -\frac{(j_{x+\Delta x}-j_x)}{\Delta x}-\frac{(j_{y+\Delta y}-j_y)}{\Delta y}-\frac{(j_{z+\Delta z}-j_z)}{\Delta z}+F$$

Allowing the time period $\Delta t$ and the volume to become infinitesimally small gives the base equation for a large family of problems in subsurface flow:

$$\frac{\partial u}{\partial t} = -\nabla\cdot\mathbf{j}+F$$

This equation appears in different forms throughout this manual. If the modeled entity $u$ is a vector, it requires a balance for every direction in space. To find a unique solution to this system, the proper initial conditions and boundary conditions must be specified.

The incompressible Navier-Stokes equations characterize the flow of freely moving fluids. This suits assessments involving liquids and gases that migrate within rivers, pipes, fractures, and streams, for example. The physics interface couples arbitrarily with other physics interfaces including the solute transport and heat transfer equations. It also links with other flow equations, which allows modeling of unusual systems including the eddying that results when ferrofluids move in the presence of a magnetic field. This physics interface is useful for flows of Newtonian fluids where the density can be assumed to be constant or nearly constant.

## *About Using the Transport of Diluted Species in Porous Media Interface*

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. The equations supply predefined options to describe mass transfer by convection (advection), dispersion, diffusion, sorption, and reactions. The convective term is defined in the mass-transport vector either with any of the momentum balances just mentioned or it can be set to a predefined velocity profile.

This physics interface describes the movements and reactions of a single solute, multiple solutes, and solutes that interact. The physics interface suits modeling of transport in saturated porous media, fluids, and even solid state diffusion, where the physics can be slow diffusion in a solid or stagnant pond, rapid transport in a fracture, or temperature-dependent reactions in multiple phases. This physics interface also covers leaching from pesticide applications and landfills as well as chemical partitioning from liquid to vapor phase. It is available in all space dimensions.

This physics interface facilitates environmental models of pollutants migrating in an aquifer and reservoir analyses involving oil flow stimulated by surfactants. It also suits assessing microbial communities and movement of dissolved oxygen in a river or waste stream.

Linking arbitrarily to and from other physics interfaces allows an unusually wide range of investigation. Links provide driving forces such as velocity and electric fields plus feedback chemical to other physics. Chemical properties and reactions can change and be changed by temperature, pressure, electric potential, magnetic potential, and shear rates. Temperature-dependent dissolution rates, exothermic and endothermic reactions, phase changes, electrochemistry, and ferrofluidics fall well inside the wide range of multiphysics processes that are straightforward to describe in a single model.

Expressions for fluid velocities can come from any flow equation in COMSOL Multiphysics, including model results and equations you write. This means you can enter a number or an expression to drive the solute transport without fully simulating the flow field.

As an example, pesticides sprayed onto crops leach into the dry soil with irrigation. The chemical plume can spread or disperse as the contaminated liquid migrates around solid grains.

## *The Subsurface Flow Module Physics Interface Guide*

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

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

In the *COMSOL Multiphysics Reference Manual*:

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

| PHYSICS INTERFACE | ICON | TAG | SPACE DIMENSION | AVAILABLE STUDY TYPE |
|---|---|---|---|---|
| **Chemical Species Transport** | | | | |
| Transport of Diluted Species | | tds | all dimensions | stationary; time dependent |

| PHYSICS INTERFACE | ICON | TAG | SPACE DIMENSION | AVAILABLE STUDY TYPE |
|---|---|---|---|---|
| Transport of Diluted Species in Porous Media |  | tds | all dimensions | stationary; time dependent |
| Transport of Diluted Species in Fractures |  | dsf | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| **Reacting Flow** |  |  |  |  |
| Laminar Flow, Diluted Species |  | — | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| **Fluid Flow** |  |  |  |  |
| **Single-Phase Flow** |  |  |  |  |
| Creeping Flow |  | spf | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| Laminar Flow[1] |  | spf | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| Phase Transport |  | phtr | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| **Porous Media and Subsurface Flow** |  |  |  |  |
| Brinkman Equations |  | br | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| Darcy's Law |  | dl | all dimensions | stationary; time dependent |
| Fracture Flow |  | esff | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| Richards' Equation |  | dl | all dimensions | stationary; time dependent |
| Multiphase Flow in Porous Media |  | — | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| Two-Phase Darcy's Law |  | tpdl | 3D, 2D, 2D axisymmetric | stationary; time dependent |

| PHYSICS INTERFACE | ICON | TAG | SPACE DIMENSION | AVAILABLE STUDY TYPE |
|---|---|---|---|---|
| Free and Porous Media Flow | | fp | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| Phase Transport in Porous Media | | phtr | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| **Heat Transfer** | | | | |
| Heat Transfer in Solids | | ht | all dimensions | stationary; time dependent |
| Heat Transfer in Fluids | | ht | all dimensions | stationary; time dependent |
| Heat Transfer in Solids and Fluids | | ht | all dimensions | stationary; time dependent |
| Heat Transfer in Porous Media | | ht | all dimensions | stationary; time dependent |
| **Structural Mechanics** | | | | |
| Poroelasticity | | poro | 3D, 2D, 2D axisymmetric | stationary; time dependent |
| [1] This physics interface is included with the core COMSOL package but has added functionality for this module. | | | | |

### *Common Physics Interface and Feature Settings and Nodes*

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

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

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

## *Subsurface Flow Module Study Availability*

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

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

## *The Liquids and Gases Materials Database*

The Subsurface Flow Module includes an additional **Liquids and Gases** material database with temperature-dependent fluid dynamic and thermal properties.

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

# Overview of the User's Guide

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

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

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### TABLE OF CONTENTS AND INDEX

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

### THE SINGLE-PHASE FLOW BRANCH

Single-Phase Flow Interfaces section describes the Laminar and Creeping Flow interfaces, and The Phase Transport Interface section describes the transport of multiple immiscible phases in free flow.

### THE POROUS MEDIA FLOW BRANCH

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

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

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

### THE CHEMICAL SPECIES TRANSPORT BRANCH

Chemical Species Transport Interfaces chapter describes the physics interfaces found under the Chemical Species Transport branch when adding a physics interface. The Transport of Diluted Species interface is used to compute the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid or solid can be computed.

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

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

### THE HEAT TRANSFER BRANCH

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

The Heat Transfer Interface models heat transfer by conduction and convection. Surface-to-ambient radiation effects around edges and boundaries can also be included. The physics interfaces are available in 1D, 2D, and 3D and for axisymmetric models with cylindrical coordinates in 1D and 2D.

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

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

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### THE STRUCTURAL MECHANICS BRANCH

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

# 2

# Single-Phase Flow Interfaces

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

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

# The Laminar Flow and Creeping Flow Interfaces

In this section:

- The Creeping Flow Interface
- The Laminar Flow Interface

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

In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings** sections, all accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

## *The Creeping Flow Interface*

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

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

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

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

#### PHYSICAL MODEL

By default, the **Neglect inertial term (Stokes flow)** check box is selected. If unchecked, the inertial terms are included in the computations.

#### DISCRETIZATION

By default, the Creeping Flow interface uses **P2+P1** elements**.** Contrary to general laminar and turbulent single-phase flow simulations employing purely linear P1+P1 elements, P2+P1 elements are well suited for most creeping flow simulations but are not in general fully conservative. Full conservation properties and high accuracy is obtained by selecting P2+P2 or P3+P3 elements.

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

#### CONSISTENT STABILIZATION

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

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

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

## The Laminar Flow Interface

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

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

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

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

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

#### SETTINGS

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

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

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

##### *About the Physics Interface Label Names*

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

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

#### PHYSICAL MODEL

##### *Compressibility*

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

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

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

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

### *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.

### *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 $p_A = p + p_{\mathrm{ref}}$, or the gauge pressure $p$. When $p_{\mathrm{ref}}$ is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also 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** $\mathbf{u}$ and its components, and the **Pressure** $p$.

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

### ADVANCED SETTINGS

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

The **Use pseudo time stepping for stationary equation form** 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.

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

### DISCRETIZATION

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

Some higher-order interpolations are also available, and 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.

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

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

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

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

[1] A feature that may require an additional license

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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.

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In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

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

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

#### *Absolute Pressure*

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

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

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

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

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

### FLUID PROPERTIES

#### *Density*

The density can either be specified by a material, or by a **User defined** expression. The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by $p_{\text{ref}}$ for weakly compressible flows and $p_{\text{ref}}$ and $T_{\text{ref}}$ 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.

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

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

## *Volume Force*

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

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

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

## *Initial Values*

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

### INITIAL VALUES

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

## *Wall*

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls.

### BOUNDARY CONDITION

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

- No Slip
- Slip
- Leaking Wall

#### *No Slip*

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

#### *Slip*

The **Slip** option prescribes a no-penetration condition, $\mathbf{u}\cdot\mathbf{n}=0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops.

From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

#### *Leaking Wall*

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

### 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, $\mathbf{u}_\mathrm{tr}$. 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 $\mathbf{u}_\mathrm{tr} = \mathbf{0}$. If the frame moves, $\mathbf{u}_\mathrm{tr}$ becomes equal to the frame movement. $\mathbf{u}_\mathrm{tr}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

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

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

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

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

#### CONSTRAINT SETTINGS

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

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

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

#### PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure. If the reference pressure $p_{\mathrm{ref}}$, defined at the physics interface level, is equal to 0, the value of the **Pressure** $p_0$, at the boundary, is the absolute pressure. Otherwise, $p_0$ is the relative pressure at the boundary.

- The **Suppress backflow** option adjusts the inlet pressure locally in order to prevent fluid from exiting the domain through the boundary. If you clear the suppress backflow option, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.

- **Flow direction** controls in which direction the fluid enters the domain.
  - For **Normal flow**, it prescribes zero tangential velocity component.
  - For **User defined**, an **Inflow velocity direction** $\mathbf{d_u}$ (dimensionless) should be specified. The magnitude of $\mathbf{d_u}$ does not matter, only the direction. $\mathbf{d_u}$ must point into the domain.

### FULLY DEVELOPED FLOW

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow towards 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**, $U_{\mathrm{av}}$.
- **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 inflow boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the inlet boundary. A fully developed flow boundary cannot be adjacent to any Interior Wall feature.

### CONSTRAINT SETTINGS

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

- Prescribing Inlet and Outlet Conditions
- Normal Stress Boundary Condition

## *Outlet*

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

### BOUNDARY CONDITION

The available **Boundary condition** options for an outlet are **Pressure, 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. If the reference pressure $p_{\mathrm{ref}}$, defined at the physics interface level, is equal to 0, the value of the **Pressure** $p_0$, at the boundary, is the absolute pressure. Otherwise, $p_0$ is the relative pressure at the boundary.

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

### VELOCITY

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

### 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**, $U_{\mathrm{av}}$.

- **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 fully developed flow condition requires any volume force to be approximately aligned with the normal of the outlet boundary. A fully developed flow boundary cannot be adjacent to any Interior Wall feature.

### CONSTRAINT SETTINGS

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

Prescribing Inlet and Outlet Conditions

## *Symmetry*

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

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

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

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

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

### BOUNDARY SELECTION

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

### CONSTRAINT SETTINGS

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

## *Open Boundary*

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

### BOUNDARY CONDITIONS

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

#### *Normal Stress*

The **Normal stress** $f_0$ condition implicitly imposes $p \approx f_0$ .

#### *No Viscous Stress*

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

The **No viscous stress** condition prescribes:

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

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

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

## *Boundary Stress*

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

### BOUNDARY CONDITION

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

#### *General Stress*

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

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

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

for the compressible and the incompressible formulations.

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

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

If $\partial u_n/\partial n$ is small, Equation 2-1 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:

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

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

for the compressible and the incompressible formulations.

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

$$p = 2\mu\frac{\partial u_n}{\partial n}+\mathrm{f}_0 \tag{2-2}$$

If $\partial u_n/\partial n$ is small, Equation 2-2 states that $p \approx \mathrm{f}_0$.

### CONSTRAINT SETTINGS

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

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

## *Periodic Flow Condition*

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

If the boundaries are curved, 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.

### PRESSURE DIFFERENCE

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

A value or expression should be specified for the **Pressure difference**, $p_{\mathrm{src}} - p_{\mathrm{dst}}$. This pressure difference can, for example, drive the fully developed flow in a channel.

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

### CONSTRAINT SETTINGS

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

### ORIENTATION OF SOURCE

For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

## *Flow Continuity*

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

A Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Flow Continuity** node, additional Fallback feature subnodes can be added.

## *Pressure Point Constraint*

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

### PRESSURE CONSTRAINT

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

### CONSTRAINT SETTINGS

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

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.

## *Point Mass Source*

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

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

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

### SOURCE STRENGTH

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

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

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

## *Line Mass Source*

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

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

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

### SELECTION

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

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

### SOURCE STRENGTH

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

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

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

## Gravity

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

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value. 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**, an edit field for the **Turbulent Schmidt number** appears. See also Theory for Buoyancy-Induced Turbulence in the *CFD Module User's Guide*.

### ACCELERATION OF GRAVITY

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

# Theory for the Single-Phase Flow Interfaces

The theory for the Single-Phase Flow, Laminar Flow interface is described in this section:

- General Single-Phase Flow Theory
- Compressible Flow
- Weakly Compressible Flow
- The Mach Number Limit
- Incompressible Flow
- The Reynolds Number
- Theory for the Wall Boundary Condition
- Prescribing Inlet and Outlet Conditions
- Fully Developed Flow (Inlet)
- Fully Developed Flow (Outlet)
- Normal Stress Boundary Condition
- Mass Sources for Fluid Flow
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- Discontinuous Galerkin Formulation
- Particle Tracing in Fluid Flow
- References for the Single-Phase Flow, Laminar Flow Interfaces

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

## *General Single-Phase Flow Theory*

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

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0 \tag{2-3}$$

$$\rho\frac{\partial\mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\tau] + \mathbf{F} \tag{2-4}$$

$$\rho C_p\left(\frac{\partial T}{\partial t} + (\mathbf{u}\cdot\nabla)T\right) = -(\nabla\cdot\mathbf{q}) + \tau{:}\mathbf{S} - \frac{T}{\rho}\frac{\partial\rho}{\partial T}\bigg|_p\left(\frac{\partial p}{\partial t} + (\mathbf{u}\cdot\nabla)p\right) + Q \tag{2-5}$$

where

- $\rho$ is the density (SI unit: kg/m$^3$)
- $\mathbf{u}$ is the velocity vector (SI unit: m/s)
- $p$ is pressure (SI unit: Pa)
- $\tau$ is the viscous stress tensor (SI unit: Pa)
- $\mathbf{F}$ is the volume force vector (SI unit: N/m$^3$)
- $C_\mathrm{p}$ is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- $T$ is the absolute temperature (SI unit: K)
- $\mathbf{q}$ is the heat flux vector (SI unit: W/m$^2$)
- $Q$ contains the heat sources (SI unit: W/m$^3$)
- $\mathbf{S}$ is the strain-rate tensor:

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

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

$$\mathbf{a}{:}\mathbf{b} = \sum_n\sum_m a_{nm}b_{nm} \tag{2-6}$$

This is sometimes referred to as the double dot product.

Equation 2-3 is the continuity equation and represents conservation of mass. Equation 2-4 is a vector equation which represents conservation of momentum. Equation 2-5 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 2-3 through Equation 2-5, constitutive relations are needed. For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

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

The dynamic viscosity, μ (SI unit: Pa·s), for a Newtonian fluid is allowed to depend on the thermodynamic state but not on the velocity field. All gases and many liquids can be considered Newtonian. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions. The Heat Transfer Module treats all fluids as Newtonian according to Equation 2-7.Other commonly used constitutive relations are Fourier's law of heat conduction and the ideal gas law.

In theory, the same equations describe both laminar and turbulent flows. In practice, however, the mesh resolution required to simulate turbulence with the Laminar Flow interface makes such an approach impractical.

There are several books where derivations of the Navier-Stokes equations and detailed explanations of concepts such as Newtonian fluids can be found. See, for example, the classical text by Batchelor (Ref. 3) and the more recent work by Panton (Ref. 4).

Many applications describe isothermal flows for which Equation 2-5 is decoupled from Equation 2-3 and Equation 2-4.

### 2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 2-3 and Equation 2-4 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 2-4. 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 2-3 and Equation 2-4 therefore assumes that

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

## Compressible Flow

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

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

and the momentum equation:

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

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, $\mathrm{Ma}$, defined by

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

where $a$ is the speed of sound. A flow is formally incompressible when $\mathrm{Ma} = 0$. This is theoretically achieved by letting the speed of sound tend to infinity. The Navier-Stokes equations then have the mathematical property that pressure disturbances are instantaneously propagated throughout the entire domain. This results in a parabolic equation system.

The momentum equation, Equation 2-9, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 2-8, 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 2-9 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.

The practical Mach number limit is lower than one, however. The main reason is that the numerical scheme (stabilization and boundary conditions) of the Laminar Flow interface does not recognize the direction and speed of pressure waves. The fully compressible Navier-Stokes equations do, for example, start to display very sharp gradients already at moderate Mach numbers. But the stabilization for the single-phase flow interface does not necessarily capture these gradients. It is impossible to give an exact limit where the low Mach number regime ends and the moderate Mach number regime begins, but a rule of thumb is that the Mach number effects start to appear at $\mathrm{Ma} = 0.3$. For this reason, the compressible formulation is referred to as *Compressible flow (Ma<0.3)* in COMSOL Multiphysics.

## *Incompressible Flow*

When the temperature variations in the flow are small, a single-phase fluid can often be assumed incompressible; that is, ρ is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant ρ, Equation 2-8 reduces to

$$\rho\nabla\cdot\mathbf{u} = 0 \tag{2-10}$$

and Equation 2-9 becomes

$$\rho\frac{\partial\mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F} \tag{2-11}$$

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:

$$\mathrm{Re} = \frac{\rho U L}{\mu}$$

where $U$ denotes a velocity scale, and $L$ denotes a representative length. The Reynolds number represents the ratio between inertial and viscous forces. At low Reynolds numbers, viscous forces dominate and tend to damp out all disturbances, which leads to laminar flow. At high Reynolds numbers, the damping in the system is very low, giving small disturbances the possibility to grow by nonlinear interactions. If the Reynolds number is high enough, the flow field eventually ends up in a chaotic state called turbulence.

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

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

## *Theory for the Wall Boundary Condition*

See Wall for the node settings.

### SLIP

The Slip condition assumes that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this is a reasonable approximation if the important effect of the wall is to prevent fluid from leaving the domain. Mathematically, the constraint can be formulated as:

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

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

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

expressing that there is no flow across the boundary and no viscous stress in the tangential direction.

For a moving wall with translational velocity $\mathbf{u}_{\mathrm{tr}}$, $\mathbf{u}$ in the above equations is replaced by the relative velocity $\mathbf{u}_{\mathrm{rel}} = \mathbf{u}-\mathbf{u}_{\mathrm{tr}}$.

#### SLIDING WALL

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

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

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

  where $\mathbf{t} = (n_y, -n_x)$ for 2D and $\mathbf{t} = (n_z, -n_r)$ for axial symmetry.
- For 3D components, the velocity is set equal to a given vector $\mathbf{u}_{\mathrm{w}}$ projected onto the boundary plane:

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

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

## *Prescribing Inlet and Outlet Conditions*

The Navier-Stokes equations can show large variations in mathematical behavior, ranging from almost completely elliptic to almost completely hyperbolic. This has implications when it comes to prescribing admissible boundary conditions. There is also a discrepancy between mathematically valid boundary conditions and practically useful boundary conditions. See Inlet and Outlet for the node settings.

### INLET CONDITIONS

An inlet requires specification of the velocity components. The most robust way to do this is to prescribe a velocity field using a Velocity condition.

A common alternative to prescribing the complete velocity field is to prescribe a pressure and all but one velocity component. The pressure cannot be specified pointwise because this is mathematically over-constraining. Instead the pressure can be specified via a stress condition:

$$-p+2\mu\frac{\partial u_n}{\partial n}=F_n \tag{2-12}$$

where $\partial u_n/\partial n$ is the normal derivative of the normal velocity component. Equation 2-12 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 2-12 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 2-12, all but one velocity component must be specified. For low Reynolds numbers, this can be specified by a vanishing tangential stress condition:

$$\mu\frac{\partial u_t}{\partial n}=0$$

which is what the Normal stress condition does. Vanishing tangential stress becomes a less well-posed inlet condition as the Reynolds number increases. The Pressure condition in the Inlet feature therefore requires a flow direction to be prescribed, which provides a well-posed condition independent of Reynolds number.

### OUTLET CONDITIONS

The most common approach is to prescribe a pressure via a normal stress condition on the outlet. This is often accompanied by a vanishing tangential stress condition:

$$\mu\frac{\partial u_t}{\partial n} = 0$$

where $\partial u_t/\partial n$ is the normal derivative of the tangential velocity field. It is also possible to prescribe $u_t$ to be zero. The latter option should be used with care since it can have a significant effect on the upstream solution.

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

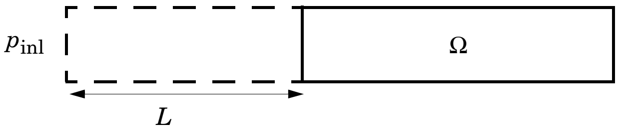
#### ALTERNATIVE FORMULATIONS

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

Normal Stress Boundary Condition

### *Fully Developed Flow (Inlet)*

The Fully Developed Flow boundary condition can be understood from the following figure:



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

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

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

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

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

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

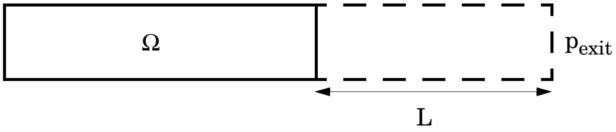
where <·> denotes the average over the inlet. Since the equation for $P_{\mathrm{inl}}$ is a DAE (the equation for $P_{\mathrm{inl}}$ does not contain $P_{\mathrm{inl}}$), it must be solved coupled to Navier-Stokes and it must be treated by a Vanka pre- and post-smoother if iterative solvers are employed.

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

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

## *Fully Developed Flow (Outlet)*

The Fully Developed Flow boundary condition can be understood from the following figure:



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

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

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

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

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

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

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the outlett can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω. The inlet pressure, $P_{\mathrm{exit}}$, must be solved for and the its equation is a discrete algebraic equation (DAE) for $P_{\text{exit}}$. 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 $P_{\text{ext}}$ is a DAE, it must be solved coupled to Navier-Stokes and it must be treated by a Vanka pre- and post-smoother if iterative solvers are employed.

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).

## *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

$$p=2\mu\frac{\partial u_n}{\partial n}+f_0 \tag{2-13}$$

If $\partial u_n/\partial n$ is small, Equation 2-13 states that $p\approx f_0$.

The Normal Stress condition is the mathematically correct version of the Pressure Conditions condition (Ref. 4), but it is numerically less stable.

## *Pressure Boundary Condition*

For single-phase flow, a mathematically correct natural boundary condition for outlets is

$$\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -p_0\mathbf{n} \tag{2-14}$$

$$(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n} \tag{2-15}$$

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 2-14 or Equation 2-15 can be supplemented with a tangential velocity condition

$$\mathbf{u}\cdot\mathbf{t} = 0 \tag{2-16}$$

If so, the no-tangential-stress condition is overridden. An issue with Equation 2-14 or Equation 2-15 is that it does not strongly enforce unidirectional flow on the boundary. If the prescribed pressure on an outlet is too high, parts of the outlet can actually have inflow. This is not as much of an issue for the Navier-Stokes equations as it is an issue for scalar transport equations solved along with the Navier-Stokes equations. Hence, when applying the **Pressure** boundary condition at an outlet or inlet you can further constrain the flow. With the Suppress backflow option

$$\begin{gathered}\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0\mathbf{n}\\ (-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -\hat{p}_0\mathbf{n}\\ \hat{p}_0 \le p_0\end{gathered}, \tag{2-17}$$

the normal stress is adjusted to keep

$$\mathbf{u}\cdot\mathbf{n} \ge 0 \tag{2-18}$$

Equation 2-17 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 2-17 does not completely prevent backflow, but the backflow is substantially reduced. Backflow is suppressed also when external forces are acting on the fluid, provided the magnitude of these forces are of the same order as the dynamic pressure at the outlet.

A pressure condition can also be applied at an inlet. In this case, either the normal stress is prescribed

$$\begin{gathered}\mathbf{n}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0\\ \mathbf{n}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -\hat{p}_0\\ \hat{p}_0 \geq p_0\end{gathered}\tag{2-19}$$

together with the tangential condition in Equation 2-16, or, a general flow direction is prescribed.

$$\begin{gathered}\mathbf{r}_{\mathbf{u}}^T\left(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_0(\mathbf{r}_{\mathbf{u}}\cdot\mathbf{n})\\ \mathbf{r}_{\mathbf{u}}^T(-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T))\mathbf{n} = -\hat{p}_0(\mathbf{r}_{\mathbf{u}}\cdot\mathbf{n})\\ \hat{p}_0 \geq p_0\\ \mathbf{u}-(\mathbf{u}\cdot\mathbf{r}_{\mathbf{u}})\mathbf{r}_{\mathbf{u}} = \mathbf{0},\ \mathbf{r}_{\mathbf{u}} = \frac{\mathbf{d}_{\mathbf{u}}}{\|\mathbf{d}_{\mathbf{u}}\|}\end{gathered}\tag{2-20}$$

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

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

## *Mass Sources for Fluid Flow*

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

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

### POINT SOURCE

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

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q} = \dot{q}_\mathrm{p} \tag{2-21}$$

An alternative way to form a point source/sink is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant, results in the same point source. For this alternative approach, effects resulting from the physical object volume, such as drag and fluid displacement, need to be neglected.

The weak contribution

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

is added to a point in the geometry. As can be seen from Equation 2-21, $\dot{Q}$ 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 2-21 corresponds to a finite pressure in a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region, but also a more extreme pressure value. It is important not to mesh too finely around a point source since the resulting pressure can result in unphysical values for the density, for example. It can also have a negative effect on the condition number for the equation system.

### LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}$ (SI unit: kg/(m$^3$·s)), located within a tube with cross-sectional area $\delta S$ and then letting $\delta S$ tend to zero, while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_\mathrm{l}$ (SI unit: kg/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_\mathrm{l} \tag{2-22}$$

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.

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

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

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

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## *Numerical Stability — Stabilization Techniques for Fluid Flow*

The momentum equation (Equation 2-9 or Equation 2-11) 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** button ( 👁 ) and select **Stabilization**.

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

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

### STREAMLINE DIFFUSION

For strongly coupled systems of equations, the streamline diffusion method must be applied to the system as a whole rather than to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 7) and were later extended to Galerkin least-squares (GLS) applied to the Navier-Stokes equations (Ref. 8). This is the streamline diffusion formulation that COMSOL Multiphysics supports. The time-scale tensor is the diagonal tensor presented in Ref. 9.

The time-scale tensors for time-dependent problems should in theory depend on a time-scale that many references just set to the time-step taken by the time-solver, $\Delta t$ (see for example Ref. 8 and Ref. 9). This simple approach doesn't 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. COMSOL Multiphysics therefore replaces $\Delta t^2$ 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. 10. 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. 8 with a shock-capturing viscosity of the Hughes-Mallet type Ref. 7.

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

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

### ISOTROPIC DIFFUSION

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

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Numerical Stabilization and Iterative in the *COMSOL Multiphysics Reference Manual*

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## Solvers for Laminar Flow

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

### NONLINEAR SOLVER

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

#### Stationary Solver

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

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

#### *Time-Dependent Solver*

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

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

### LINEAR SOLVER

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

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

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

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

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

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

- In the *COMSOL Multiphysics Reference Manual:*Time-Dependent Solver
- Multigrid, Direct, Iterative, SCGS, SOR Line, and Vanka
- Stationary Solver

### *Pseudo Time Stepping for Laminar Flow Models*

A stationary formulation has per definition no time derivatives and Equation 2-11 reduces to:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]+\mathbf{F} \tag{2-23}$$

Solving Equation 2-23 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 2-23:

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

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

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

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

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

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

The default manual expression is

$$\begin{gathered}1.3^{\min(\text{niterCMP},\,9)}+\\ \text{if}(\text{niterCMP}>20,\,9\cdot 1.3^{\min(\text{niterCMP}-20,\,9)},\,0)+\\ \text{if}(\text{niterCMP}>40,\,90\cdot 1.3^{\min(\text{niterCMP}-40,\,9)},\,0)\end{gathered}\tag{2-24}$$

The variable `niterCMP` is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. $\text{CFL}_{\text{loc}}$ starts at $1.3$ and increases by 30% each iteration until it reaches $1.3^9\approx 10.6$ . It remains there until iteration number 20 at which it starts to increase until it reaches approximately $106$. A final increase after iteration number 40 then takes it to $1060$. Equation 2-24 can, for some advanced flows, increase $\text{CFL}_{\text{loc}}$ too slowly or too quickly. $\text{CFL}_{\text{loc}}$ can then be tuned for the specific application.

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

### *Discontinuous Galerkin Formulation*

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

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

The formulation used in the Fluid Flow interfaces in COMSOL Multiphysics is the Symmetric Interior Penalty Galerkin method (SIPG). The SIPG method can be regarded to satisfy the boundary conditions in an integral sense rather than pointwise. More information on SIPG can be found in Ref. 14.

In particular, the SIPG formulation includes a penalty parameter that must be large enough for the formulation to be coercive. The higher the value, the better the boundary condition is fulfilled, but a too high value results in an ill-conditioned equation system. The penalty parameter in COMSOL Multiphysics is implemented according to Ref. 15.

## *Particle Tracing in Fluid Flow*

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

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

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

where $\mathbf{x}$ is the position of the particle, $m$ the particle mass, and $\mathbf{F}$ is the sum of all forces acting on the particle. Examples of forces acting on a particle in a fluid are the drag force, the buoyancy force, and the gravity force. The drag force represents the force that a fluid exerts on a particle due to a difference in velocity between the fluid and the particle. It includes the viscous drag, the added mass, and the Basset history term. Several empirical expressions have been suggested for the drag force. One of those is the one proposed by Khan and Richardson (Ref. 12). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

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

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

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

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

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# 3

# 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 ( ).

- Modeling Porous Media and Subsurface Flow
- The Darcy’s Law Interface
- The Richards’ Equation Interface
- The Two-Phase Darcy’s Law Interface
- The Phase Transport Interface
- The Multiphase Flow in Porous Media Interface
- The Fracture Flow Interface
- The Brinkman Equations Interface
- The Free and Porous Media Flow Interface
- Theory for the Darcy’s Law Interface
- Theory for the Brinkman Equations Interface
- Theory for the Fracture Flow Interface
- Theory for the Richards’ Equation Interface
- Theory for the Two-Phase Darcy’s Law Interface
- Theory for the Phase Transport Interface
- Theory for the Multiphase Flow in Porous Media Interface

# Modeling Porous Media and Subsurface Flow

The Fluid Flow physics features included with the Subsurface Flow Module are used to characterize movements of liquids, gases, and other flowing media, such as molten rock.

The **Porous Media and Subsurface Flow** branch ( ) contains physics interfaces for the following sets of equations that apply under different conditions.

- The Darcy's Law Interface describes low-velocity flows of one or more fluids.
- The Richards' Equation Interface governs the wetting and drying of rocks or soils.
- The Two-Phase Darcy's Law Interface describes two-phase fluid movement through interstices in a porous medium. An extra equation is computed to calculate the saturation transport.
- The Fracture Flow Interface is a variant of Darcy's law that defines the flow along the interior boundaries representing fractures within a porous (or solid) medium.
- The Brinkman Equations Interface is for porous media high-velocity flows.
- The Free and Porous Media Flow Interface combines free flow adjacent to porous domains.
- The Laminar Flow and Creeping Flow Interfaces are available with all COMSOL licenses and use the *Navier-Stokes equations* to describe free flows within a river or well, for example.

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.

## *Selecting the Right Fluid Flow Interface for Porous Media*

To model fluid flows in porous media, use either Darcy's Law or the Brinkman Equations interface. Darcy's law is preferable when the major driving force for the flow is the pressure gradient, and the momentum transfer by shear stresses within the fluid is negligible. This is usually true in the case of low permeability in the porous medium.

The corresponding physics interfaces combine arbitrarily and link to other physics including solute transport, heat transfer, electric potentials, magnetic potentials, and structural deformation, to name a few. Because any expression can be entered for coefficients like permeability or density, the equations set up in this module are especially flexible.

Figure 3-1 illustrates typical settings where the various flow regimes apply.

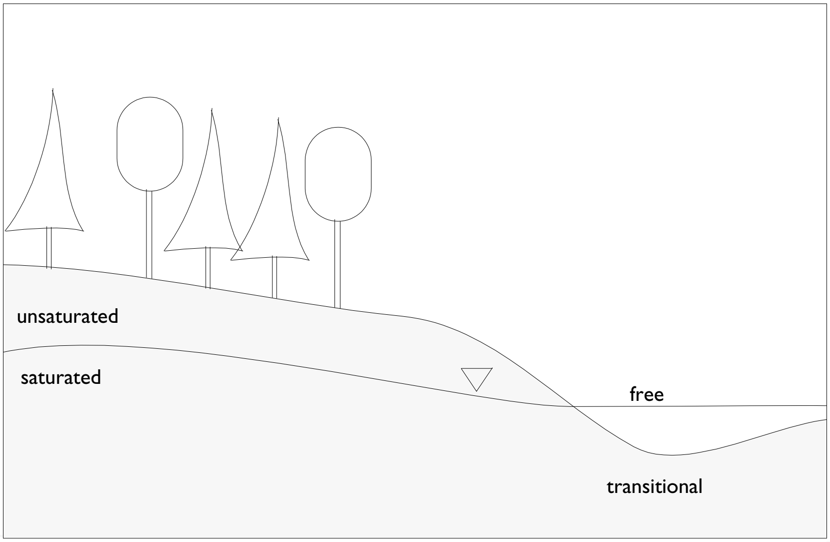

*Figure 3-1: Vertical cross section through ground near a river. Labels indicate flow regimes. The triangle denotes the water table.*

The Single-Phase Flow, Laminar Flow interface uses Navier-Stokes equations for flows of liquids and gases moving freely in pipes, channels, caves, and rivers. These equations detail fluid movements through the intricate networks of pores and cracks in porous media. The scale of interest in most geologic problems, however, makes solving for velocity profiles within pores unfeasible owing to the sheer volume of the data required and machine constraints on computational effort.

The Porous Media and Subsurface Flow interfaces — Darcy’s Law, Brinkman Equation, and Richards’ Equation — circumvent detailing flow in each pore. Instead these equations estimate flow rates by lumping the properties of the solid grains and the spaces between them in representative volumes.

The Fluid Flow interfaces in this module can be grouped according to driving forces. Consider Bernoulli's equation for mechanical energy along a streamline in inviscid fluids:

$$\frac{d}{ds}\left(\frac{1}{2g}u^2\right)+\frac{1}{\rho_\mathrm{f}g}\frac{d}{ds}p+\frac{d}{ds}D = \mathrm{const.}$$

Here $s$ represents a location on the streamline, $u$ denotes the fluid velocity, $\rho_\mathrm{f}$ is the fluid density, $p$ refers to the fluid pressure, $g$ represents gravity, and $D$ is the elevation. The Bernoulli equation states that the total mechanical energy is constant along the fluid trajectory in a steady flow system. Moreover, the energy can shift between velocity, pressure, and elevation along the streamline.

With the extended Laminar Flow interface and the Brinkman Equations, all the driving forces are non-negligible. When solved, the equations give the directional fluid velocities and the pressure; elevation is a coordinate in the model. With Darcy's Law and Richards' Equation, the momentum is so small it can be neglected. Pressure alone drives the flow for these physics interfaces.

# The Darcy's Law Interface

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

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

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

### SETTINGS

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

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

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

### 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.

Enter a value for the acceleration of gravity. The default is taken from the predefined physical constant `g_const`, which is the standard acceleration of gravity.

### PHYSICAL MODEL

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

### DEPENDENT VARIABLES

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

### DISCRETIZATION

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

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*.

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

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*Terzaghi Compaction*: Application Library path **Subsurface_Flow_Module/Flow_and_Solid_Deformation/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 available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

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

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

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

### DOMAIN

- Fluid and Matrix Properties
- Storage Model
- Mass Source
- Poroelastic Storage
- Richards' Equation Model
- Gravity
- Initial Values

### BOUNDARY, EDGE, AND POINT

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

- Atmosphere/Gauge
- Cross Section
- Thickness
- Flux Discontinuity
- Fracture Flow
- Hydraulic Head
- Inlet
- Interior Wall
- Mass Flux
- No Flow
- Outlet
- Pervious Layer
- Pressure
- Pressure Head
- 1
- 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.

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

- Pressure
- Pressure Head
- Hydraulic Head
- Interior Wall
- Pervious Layer
- Flux Discontinuity
- Fracture Flow
- Thin Barrier

## *Fluid and Matrix Properties*

The **Fluid and Matrix Properties** node adds the equations for Darcy's law, Equation 3-1 and Equation 3-13 (excluding any mass sources), and contains settings for the fluid properties and the porous matrix properties such as the effective porosity.

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_{\mathrm{m}} \tag{3-1}$$

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) \tag{3-2}$$

### FLUID PROPERTIES

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

*Density*

The default **Density** $\rho$ (SI unit: $\mathrm{kg/m^3}$) uses values **From material** based on the **Fluid material** selection.

- For **User defined** enter another value or expression. The default is 0 $\mathrm{kg/m^3}$.
- For **Ideal gas** it uses the ideal gas law to describe the fluid. In this case, specify the thermodynamics properties. Select a **Gas constant type**—**Specific gas constant** $R_s$ (the default) or **Mean molar mass** $M_n$ (SI unit: J/(mol·K)). For **Mean molar mass** the universal gas constant $R$ = 8.314 J/(mol·K) is used as the built-in physical constant. For both properties, the defaults use values **From material**. For **User defined** enter another value or expression.

#### *Dynamic Viscosity*

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

If **Hydraulic conductivity** is selected as the **Permeability model** under the **Matrix Properties** section, the settings for the dynamic viscosity are unavailable. The hydraulic conductivity is defined using a combination of fluid and matrix properties and replaces the need to define the dynamic viscosity.

### MATRIX PROPERTIES

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

The default **Porosity** $\varepsilon_\mathrm{p}$ (a dimensionless number between 0 and 1) uses the value **From material**, defined by the **Porous material** selected. For **User defined** the default is 0.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow—**Permeability** to define the permeability of the porous matrix, **Hydraulic conductivity** to define a combination of fluid permeability and dynamic viscosity, or **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter.

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

For **Hydraulic conductivity** $K$ (SI unit: m/s) select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.

For **Kozeny-Carman**, enter the mean particle diameter $d_\mathrm{p}$ (SI unit: m), the default value is 0.5 mm.

## *Mass Source*

The **Mass Source** node adds a mass source $Q_\mathrm{m}$, which appears on the right-hand side of the Darcy's Law equation (Equation 3-3, the equation for porosity).

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

For The Fracture Flow Interface the mass source is applicable to the right-hand side of Equation 3-6 (where it is multiplied with the fracture thickness).

### MASS SOURCE

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

## *Initial Values*

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

You can specify the pressure either directly or as an expression for the pressure head, $H_p$, or the hydraulic head, $H$; the hydraulic head and the pressure head relate to the pressure $p$ as

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

where ρ is the fluid density (SI unit: kg/m$^3$); $g$ denotes the acceleration of gravity (SI unit: m/s$^2$); and $D$ is the elevation head (SI unit: m), which is a vector in the direction over which $g$ acts.

### INITIAL VALUES

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

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.

## *Storage Model*

The **Storage Model** node adds Equation 3-13 and Equation 3-18 (excluding any mass sources). Use it to define the fluid and porous media properties, including a storage term for the specific storage.

### 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**, and for The Fracture Flow Interface, enter a value or expression for **Storage** $S$ (SI unit: 1/Pa) ($S_\mathrm{f}$ in Equation 3-6).
- For **Linearized storage** it uses the following linear equation to define the storage:

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

  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** $\chi_\mathrm{f}$ (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** $\chi_\mathrm{p}$ (SI unit: 1/Pa). The default is $1 \cdot 10^{-4}$ 1/Pa).

### FRACTURE FLOW

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

*Discrete Fracture*: Application Library path
**Subsurface_Flow_Module/Fluid_Flow/discrete_fracture**

## *Richards' Equation Model*

The **Richards' Equation Model** node defines the storage and retention models in variably saturated porous media. See the Richards' Equation Model described for the Richards' Equation interface.

## *Poroelastic Storage*

The **Poroelastic Storage** node adds Equation 3-13 and Equation 3-18 (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.

#### 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 unit: 1/Pa). The default uses values **From material** as defined by the **Fluid material** selected. For **User defined** the default is $4{\cdot}10^{-10}$ 1/Pa.

#### MATRIX PROPERTIES

The settings are the same as in the Matrix Properties section under Fluid and Matrix Properties.

## *Gravity*

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. This action will add a **Gravity** node, and gravity forces will be applied to all selected domains.

#### 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 the elevation.

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

- For 3D and 2D axisymmetric models, the default value is `-g_const` in the $z$ direction.
- For 2D models, the default value is `-g_const` in the $y$ direction.

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

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

## *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).

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** button ( ) and select **Advanced Physics Options**.

Pressure constraint on edges are available for use with the Fracture Flow boundary condition, which needs conditions on the edges surrounding the fracture-flow boundary. In other cases, pressure constraints on edges are not implemented.

## *Mass Flux*

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

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

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

For modeling mass flux from very thin objects add a **Line Mass Source** or a **Point Mass Source** node.

The **Line Mass Source** node adds mass flow originating from a tube of infinitely small radius. It is available for edges in 3D geometries or points in 2D and 2D axisymmetric geometries.

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

### MASS FLUX

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

## *Inlet*

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

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

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.

### INLET

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

## *Symmetry*

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

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

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

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 impervious boundaries. The mathematical formulation is:

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

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

## *Flux Discontinuity*

Use the **Flux Discontinuity** node to specify a mass flux discontinuity through an interior boundary. The condition is represented by the following equation:

$$-\mathbf{n}\cdot(\rho\mathbf{u}_1-\rho\mathbf{u}_2) = N_0$$

In this equation, $\mathbf{n}$ is the vector normal (perpendicular) to the interior boundary, $\rho$ is the fluid density, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the Darcy velocities in the adjacent domains (as defined in Equation 3-4) and $N_0$ is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \qquad (3\text{-}4)$$

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

### MASS FLUX

Enter a value or expression for the **Inward mass flux** $N_0$ (SI unit: kg/(m$^2$·s)). A positive value of $N_0$ represents a mass flux discontinuity in the opposite direction to the normal vector of the interior boundary.

## *Outlet*

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

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

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

#### OUTLET

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

## *Cross Section*

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

#### CROSS SECTION

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

## *Thickness*

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

#### THICKNESS

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

## *Interior Wall*

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

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

## Thin Barrier

The **Thin Barrier** boundary condition 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** $d_{\mathrm{b}}$ (SI unit: m, the default is 0.1 m) and for the **Permeability** $\kappa_{\mathrm{b}}$ (SI unit: m$^2$). The default **Permeability** $\kappa_{\mathrm{b}}$ uses the value **From material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to define a tensor value and enter another value or expression in the field or matrix.

## Pressure Head

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

### PRESSURE HEAD

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

### CONSTRAINT SETTINGS

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

## 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** button ( 👁 ) and select **Advanced Physics Options**.

## *Atmosphere/Gauge*

The **Atmosphere/Gauge** node specifies an atmospheric pressure or gauges the pressure to the atmospheric value. This means that the total hydraulic potential reduces to the gravitational pressure at the free surface. At a free surface, such as a spring or a seepage face, the pressure is atmospheric. If the pressures in the model is gauged to the atmospheric value ($p = 0$), the total hydraulic potential reduces to the gravitational potential at the free surface—for example, the height of the free surface multiplied by the fluid weight, or $\rho_f g D$. This boundary condition sets the pressure at the boundary to zero and $p = 0$.

### CONSTRAINT SETTINGS

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

## *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:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) = \rho R_\mathrm{b}\left[\frac{(p_\mathrm{b} - p)}{\rho g} + (D_\mathrm{b} - D)\right] \qquad (3\text{-}5)$$

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

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

$$\mathbf{n} \cdot \rho K \nabla (H_p + D) = \rho R_\mathrm{b}[(H_{p\mathrm{b}} - H_p) + (D_\mathrm{b} - D)] \qquad (3\text{-}6)$$

$H_\mathrm{pb}$ 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:

$$\mathbf{n}\cdot\rho K\nabla H = \rho R_{\mathrm{b}}[H_{\mathrm{b}} - H] \tag{3-7}$$

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

$K$ in Equation 3-6 and Equation 3-7 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 $D$.

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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.

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#### 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** $R_{\mathrm{b}}$ (SI unit: 1/s).

- For **Pressure and elevation** enter an **External pressure** $p_{\mathrm{b}}$ (SI unit: Pa) and **External elevation** $D_{\mathrm{b}}$ (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** $D_{\mathrm{b}}$ (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.

#### WELL

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

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

### *Fracture Flow*

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

# 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**. **Richards' Equation Model** (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 `dl`.

### GRAVITY EFFECTS

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

Enter a value for the acceleration of gravity. The default is taken from the predefined physical constant `g_const`, which is the standard acceleration of gravity.

Under **Acceleration of gravity**, enter the value for the acceleration of gravity (SI unit m/s$^2$). The default value is taken from the constant `g_const`.

### PHYSICAL MODEL

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

### DEPENDENT VARIABLES

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

### DISCRETIZATION

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

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

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

The Richards' Equation Interface has the same domain, boundary, edge, and point nodes described for The Darcy's Law Interface. The exception is Richards' Equation Model, which is described in this section.

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

## *Richards' Equation Model*

The **Richards' Equation Model** node adds Richards' equation (Equation 3-26) for flow in variably saturated porous media and provides an interface for defining the fluid properties as well as the retention model. The source term can be included as separate feature.

### FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

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

The default **Dynamic viscosity** μ (SI unit: Pa·s) uses values **From material** based on the **Fluid material** selected. For **User defined** enter another value or expression. The default is 0 Pa·s.

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

### MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** (the material defined for the domain) for the porous matrix. Select another material as needed.

#### *Permeability Model*

Select a **Permeability model** to specify the capacity of the porous material to transmit flow. Select **Permeability** to define the permeability of the porous matrix, **Hydraulic conductivity** to define a combination of fluid permeability and dynamic viscosity, or **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter.

- For **Permeability** $\kappa_s$ (SI unit: m$^2$) the default uses values **From material** as defined by the **Porous material** selected. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to enter a tensor value.
- For **Hydraulic conductivity** $K_s$ (SI unit: m/s) enter a value or expression. Select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to enter a tensor value.
- For **Kozeny-Carman**, enter a value or expression for the mean particle diameter $d_p$ (SI unit: m), the default value is 0.5 mm.

### *Saturated Liquid Volume Fraction*

The property that defines the pore volume in Richards' Equation is the **Saturated liquid volume fraction** $\theta_s$. Enter a value, which is a fraction (a dimensionless number between 0 and 1). The default is 0.25.

### *Residual Liquid Volume Fraction*

If there is a residual volume of liquid that cannot move through the pore network, also enter a **Residual liquid volume fraction** $\theta_r$. Enter a value, which is a fraction (a dimensionless number between 0 and 1). The default is 0.

## STORAGE MODEL

Select a **Storage model** $S$ (SI unit: 1/Pa) — **Linearized storage** or **User defined**. For **User defined** enter a **Storage** $S$ (SI unit: 1/Pa) value or expression. Select **Linearized storage** to use the following linear equation to define the storage:

$$S = \theta_s \chi_f + (1 - \theta_s)\chi_p$$

This expression is equivalent to the Reuss average of the fluid and solid compressibilities. Enter the value or expression for these properties to define the linear storage — **Compressibility of fluid** $\chi_f$ (SI unit: 1/Pa) and **Effective compressibility of matrix** $\chi_p$ (SI unit: 1/Pa).

## RETENTION MODEL

Select a **Retention model** — **van Genuchten**, **Brooks and Corey**, or **User defined**.

Select **van Genuchten** to use the retention model according to van Genuchten (see Equation 3-27). Then enter the values for these **Constitutive relation constants**. The constitutive parameter $m$ is equal to $1 - 1/n$.

- $\alpha$ (default is 1, and the SI unit is 1/m).
- $n$ (default is 2)
- $l$ (default is 0.5)

Select **Brooks and Corey** to use the retention model according to Brooks and Corey (see Equation 3-28). The same parameters as for the van Genuchten model also define the Brook and Corey model: $\alpha$, $n$, and $l$.

Select **User defined** to specify a retention model in Equation 3-26, instead of van Genuchten (Equation 3-27) or Brooks and Corey (Equation 3-28) models:

- **Unsaturated condition** un. The default is 0.
- **Liquid volume fraction** $\theta$. The default is $\theta_s$ (the `thetas` variable).

- **Effective saturation** $S_{\mathrm{e}}$. The default is $0$.
- **Specific moisture capacity** $C_{\mathrm{m}}$ (SI unit: $1/\mathrm{m}$). The default is $0\ (1/\mathrm{m})$.
- **Relative permeability** $k_{\mathrm{r}}$. The default is $1$.

### *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.

# The Two-Phase Darcy's Law Interface

The **Two-Phase Darcy's Law (tpdl)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It solves Darcy's law for the total pressure and the transport of the fluid content for one fluid phase. The physics interface can be used to model low velocity flows or media where the permeability and porosity are very small, for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. The physics interface can be used for stationary and time-dependent analyses.

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

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

### SETTINGS

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

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

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

### PHYSICAL MODEL

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

### DEPENDENT VARIABLES

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

### CONSISTENT STABILIZATION

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

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

### DISCRETIZATION

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

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

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

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

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

- Fluid and Matrix Properties
- Inlet
- Initial Values
- Symmetry
- Interior Wall
- Mass Flux
- No Flux
- Outlet
- Pressure and Saturation

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

## *Fluid and Matrix Properties*

The **Fluids and Matrix Properties** node adds Equation 3-16 and Equation 3-9 and defines properties including density, dynamic viscosity, relative permeability, and porosity.

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

$$\frac{\partial}{\partial t}(c_1\varepsilon_p) + \nabla\cdot(c_1\mathbf{u}) = \nabla\cdot D_c\nabla c_1 \tag{3-9}$$

### CAPILLARY MODEL

The list defaults to **Capillary diffusion** or choose **Capillary pressure**.

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

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

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

### FLUID 1 PROPERTIES

Select the material to use for **Fluid 1**. Select **Domain material** (the default value) to use the material defined for the domain. Select another material to use that material's properties.

Define the properties for **Fluid 1**:

The default **Density** $\rho_1$ (SI unit: kg/m$^3$) uses values **From material** based on the **Fluid 1** selection. For **User defined** enter another value or expression. The default is 0 kg/m$^3$.

Select a **Dynamic viscosity** $\mu_1$ (SI unit: Pa·s). The default uses values **From material** as defined by the **Fluid 1** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

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

#### FLUID 2 PROPERTIES

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

#### MATRIX PROPERTIES

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

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

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

### *Initial Values*

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

#### INITIAL VALUES

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

## *No Flux*

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

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

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

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

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

## *Pressure and Saturation*

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

### PRESSURE AND SATURATION

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

## *Mass Flux*

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

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

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

### MASS FLUX AND SATURATION

Enter a value or expression for the **Inward mass flux** $N_0$ (SI unit: kg/(m$^2$·s)). A positive value of $N_0$ represents an inward mass flux, whereas a negative value represents an outward mass flux.

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

## *Inlet*

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

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

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

### INLET

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

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

## *Outlet*

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

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

where $D_c$ is the capillary diffusion (SI unit: $m^2/s$) and $c_1 = s_1\rho_1$ is the fluid 1 content (SI unit: $kg/m^3$). This means that the normal gradient of fluid saturation does not change through this boundary.

### PRESSURE

Enter a value or expression for the **Pressure** $p$. The default value is 0. If the reference pressure $p_{\mathrm{ref}}$, defined at the physics interface level is 0, enter the absolute pressure. Otherwise, enter the relative pressure.

### *Symmetry*

The **Symmetry** node describes a symmetry boundary where there is no tangential flow. The following condition implements the symmetry condition on an axis or a flow divide:

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

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

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

### *Interior Wall*

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

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

### *Thin Barrier*

The **Thin Barrier** boundary condition can only be applied on interior boundaries.

It is similar to the **Interior Wall** boundary available on interior boundaries except that it allows pressure and concentration gradients across the boundary. The **Thin Barrier** boundary condition can be used to avoid meshing thin permeable structures by applying flux condition on interior curves and surfaces instead.

# The Phase Transport Interface

The **Phase Transport (phtr)** interface ( ), found under the **Fluid Flow > Multiphase Flow** branch ( ), when adding a physics interface, is used to simulate the transport of multiple immiscible phases either in free flow or in flow through a porous medium. This interface solves for the averaged volume fractions (also called saturations in a porous medium) of the phases, and does not track the interfaces between the different phases, although microscopic interfacial effects are taken into account in the macroscopic equations for phase transport in porous media through the capillary pressure functions. The **Phase Transport** interface can be used for stationary and time-dependent analyses.

The main feature is the **Phase and Transport Properties** node, which provides an interface for defining the phase material along with the transporting flow properties.

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

### SETTINGS

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

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

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

### PHASES

Select the volume fraction of the phase that this physics interface solves for using the volume constraint in equation Equation 3-10 (that is, its value comes from the fact that the sum of all volume fractions must equal 1). In the **From volume constraint** list, select the volume fraction of the preferred phase. By default, the first volume fraction is used:

$$s_1 = 1 - \sum_{i=2}^{N} s_i \tag{3-10}$$

### CONSISTENT AND INCONSISTENT STABILIZATION

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

There are two consistent stabilization methods: **Streamline diffusion** and **Crosswind diffusion**. 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.

There is one inconsistent stabilization method: **Isotropic diffusion**. This method is equivalent to adding a diffusion term to the equations in order to dampen the effect of oscillations by making the system somewhat less dominated by convection. By default, the **Isotropic diffusion** check box is not selected because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. If required, select the **Isotropic diffusion** check box and enter a **Tuning parameter** as a scalar positive value. The default value is 0.25. A higher value adds more isotropic diffusion.

### GRAVITY EFFECTS

When the **Include gravity** check box is selected, a global **Gravity** feature is shown in the interface model tree, and the gravitational force is added to the phase transport equations in porous domains. For more information, see Gravity.

### QUADRATURE SETTINGS

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

These settings affect the numerical integration, and you do not normally need to change them. The **Use automatic quadrature settings** check box is selected by default, meaning that the settings are taken from the main equation in the interface.

If the check box is cleared, the following setting become available:

#### *Integration Order*

The **Integration order** specifies the desired accuracy of integration during discretization. Polynomials of at most the given integration order are integrated without systematic errors. For smooth constraints, a sufficient integration order is typically twice the order of the shape function. For example, the default integration order for linear elements is 2. The integration order is a positive integer.

The settings in this section currently only affect the integration order in the **Phase and Transport Properties** and **Phase and Porous Media Transport Properties** domain features.

### DISCRETIZATION

To see all settings available in this section, click the **Show** button ( ) and select **Advanced Physics Options**. By default, the shape functions used for the volume fractions are linear.

The **Value type when using splitting of complex variables** setting should in most pure mass transport problems be set to **Real** which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

### DEPENDENT VARIABLES

Add or remove volume fractions of different phases in the model and also change the names of the dependent variables that represent the volume fractions.

Specify the **Number of phases**. There must be at least two phases. To add a single phase, click the **Add volume fraction** button ( + ) under the table. To remove a volume fraction, select it in the list and click the **Remove volume fraction** button ( ) under the table. Edit the names of the phases directly in the table.

## *The Phase Transport in Porous Media Interface*

The **Phase Transport in Porous Media** interface ( ), found under the **Fluid Flow > Porous Media and Subsurface Flow** branch ( ), is used to simulate the transport of multiple phases either in free flow or in flow through a porous medium. The interface is the same as the **Phase Transport** interface but it uses other defaults: a **Phase and Porous Media Transport Properties** node is added by default, instead of a **Phase and Transport Properties** node.

This interface is dedicated to modeling transport of multiple immiscible phases in a porous medium, taking into account their relative permeabilities and capillary pressures.

The **Phase Transport in Porous Media** interface can be used for stationary and time-dependent analyses.

The main feature is the **Phase and Porous Media Transport Properties** node, which provides an interface for defining the phase materials along with the transporting porous medium flow properties.

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

#### SETTINGS

The rest of the settings are the same as for the **Phase Transport** interface.

## *Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces*

The **Phase Transport** and **Phase Transport in Porous Media** interfaces have the following domain, boundary, edge, and point nodes (listed in alphabetic order) available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- Gravity
- Initial Values
- Interior Wall
- Mass Flux
- Mass Source
- No Flux
- Outflow
- Phase and Porous Media Transport Properties
- Phase and Transport Properties
- Porous Medium Discontinuity
- Volume Fraction

## *Phase and Transport Properties*

For this node, the Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu.

#### VELOCITY FIELD

Specify the velocity field for each phase that is not computed from the volume constraint. Select the source of the Velocity field. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a fluid flow interface added to the model component. These physics interfaces are available for selection in the velocity field list.

#### DENSITY

Enter the **Density** $\rho$ (SI unit: kg/m$^3$) of each phase. The default value is 1000 kg/m$^3$.

### *Turbulent Mixing*

This subnode is available from the context menu (right-click the Phase and Transport Properties parent node) as well as from the **Physics** toolbar, **Attributes** menu. Use this node to account for the turbulent mixing caused by the eddy diffusivity. An example is when the specified velocity field corresponds to a RANS solution.

#### TURBULENT MIXING PARAMETERS

Some physics interfaces provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** $\nu_T$ list. The list always contains the **User defined** option where any value or expression can be entered.

The default **Turbulent Schmidt number** $\mathrm{Sc}_T$ is 0.71 (dimensionless).

#### FURTHER READING

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

### *Phase and Porous Media Transport Properties*

Use this node to model the transport of multiple phases through a porous medium. The node contains functionality to include the effects of the relative permeabilities and capillary pressures.

#### MODEL INPUT

Enter the absolute pressure field (SI unit: Pa) for the phase that is computed from the volume constraint. The volumetric flux of this phase is computed using Darcy's law, and in many cases that pressure field will be computed for in a **Darcy's Law** interface, coupled to the **Phase Transport** interface using a **Multiphase Flow in Porous Media** multiphysics coupling node.

The volumetric fluxes of the other phases are also computed using Darcy's law, taking into account the relative permeabilities and capillary pressures.

### CAPILLARY PRESSURE

Select a **Capillary pressure model**—**User defined** (the default), **van Genuchten**, or **Brooks and Corey**. The latter two 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** $p_{\mathrm{c}}$ (SI unit: Pa) for the phases that are not computed from the volume constraint. The pressure of the corresponding phase is equal to the pressure of the phase computed from the volume constraint (supplied in the **Pressure** input field) plus the capillary pressure supplied for this phase.

- For **van Genuchten**, select the **Wetting phase** and enter an **Entry capillary pressure** $p_{\mathrm{ec}}$ (SI unit: Pa), the **Constitutive relations constant** $m_{\mathrm{vG}}$ (dimensionless), and **Constitutive relations constant** $l_{\mathrm{vG}}$ (dimensionless).
- For **Brooks and Corey**, select the **Wetting phase** and enter an **Entry capillary pressure** $p_{\mathrm{ec}}$ (SI unit: Pa) and the **Pore size distribution index** $\lambda_{\mathrm{p}}$ (dimensionless).

### PHASE PROPERTIES

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

Enter the **Density** $\rho$ (SI unit: kg/m$^3$), **Dynamic viscosity** $\mu$ (SI unit: Pa·s) and **Relative permeability** $\kappa_{\mathrm{r}}$ (a dimensionless number between 0 and 1) for each phase. The defaults for the **Density** and **Dynamic viscosity** are **From material,** and **User defined** for the **Relative permeability.** For **User defined,** the default values are $1000$ kg/m$^3$, $0.001$ Pa·s. and $s_i^2$ , respectively.

The **Relative permeability** input fields are only available when the **Capillary pressure model** is set to **User defined**. 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** $s_{\mathrm{r}i}$ (dimensionless, default value 0) for each phase.

### MATRIX PROPERTIES

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

The default **Porosity** $\varepsilon_p$ (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: $m^2$) uses the value **From material**, as defined by the **Porous material** selected. For **User defined** the default is the **Isotropic** scalar value of `1e-9` $m^2$. To define a tensor value, select **Diagonal**, **Symmetric**, or **Anisotropic**, and enter values or expressions in the matrix.

## *Gravity*

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Gravity Effects** settings. It defines the gravity forces from the **Gravity vector** value. Note that this feature only has an effect in porous domains.

### GRAVITY

Enter the components of the **Gravity vector** $\mathbf{g}$ . The default value is `g_const` which is the physical constant having the value 9.8066 $m/s^2$.

- For 3D and 2D axisymmetric models, the default value is `-g_const` in the $z$ direction.
- For 2D models, the default value is `-g_const` in the $y$ direction.

## *Initial Values*

The **Initial Values** node specifies the initial values for the volume fraction of each phase. These serve as an initial guess for a stationary solver or as initial condition for a transient simulation.

### DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

### INITIAL VALUES

Enter a value or expression in the field for the volume fraction of each phase except for the one computed from the volume constraint.

## *Mass Source*

In order to account for consumption or production of the different phases due to one or more reactions or other physical processes, the **Mass Source** node adds source terms to the right-hand side of the phase transport equations.

### MASS SOURCE

Add an expression for the mass source for each individual phase present, except for the one computed from the volume constraint. The net mass source of all phases together is assumed to be zero, which means that the mass is transfered to or from the phase that is computed from the volume constraint.

Select the **Mass transfer to other phases** check box if mass is transfered from or to phases not accounted for in the phase transport interface, for instance when mass is released or absorbed by the solid part of the porous matrix. In this case the mass source for the phase calculated from the volume constraint should also be specified. The net mass transfer corresponds to the sum of the mass sources for all phases and should be accounted for in the computation of the flow field.

## *No Flux*

This node is the default boundary condition on exterior boundaries. It represents boundaries where no mass flows in or out of the boundaries. Hence, the total flux is zero.

## *Volume Fraction*

This node adds a boundary condition for the volume fractions of the different phases. Set the volume fractions of all phases except the one computed from the volume constraint. This ensures that the sum of the volume fractions is equal to one.

### VOLUME FRACTION

Specify the volume fraction for each phase individually. Select the check box for the phases to specify the volume fraction, and enter a value or expression in the corresponding field. To use another boundary condition for a specific phase, click to clear the check box for the volume fraction of that phase.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

## *Mass Flux*

The **Mass Flux** node can be used to specify the total mass flux of a phase across a boundary. Set the mass flux for all phases except the one computed from the volume constraint. This ensures that the sum of the volume fractions is equal to one.

For modeling mass flux from very thin objects add a **Line Mass Source** or a **Point Mass Source** node.

The **Line Mass Source** node adds mass flow originating from a tube of infinitely small radius. It is available for edges in 3D geometries or points in 2D and 2D axisymmetric geometries.

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

### MASS FLUX

Specify the inward mass flux for each phase individually. Select the check box for the phase to prescribe a mass flux and enter a value or expression for the flux in the corresponding field. To use another boundary condition for a specific phase, click to clear the check box for the flux of that phase. Use a positive value for an inward flux. The units are based on the geometric entity: **Boundaries**: (SI unit: $\mathrm{kg/(m^2 \cdot s)}$), **Lines** (SI unit: $\mathrm{kg/(m \cdot s)}$, and **Points** (SI unit: kg/s)).

## *Outflow*

Set this condition at exterior boundaries where the phases are transported out of the model domain by fluid motion. The outward mass flux for each phase is in this case set to the normal outward phase velocity times the phase density.

## *Interior Wall*

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

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

## *Porous Medium Discontinuity*

The **Porous Medium Discontinuity** boundary condition can only be applied on interior boundaries, and only when on both sides of the boundary a **Phase and Porous Media Transport Properties** domain condition is active. Set this condition at boundaries over which the capillary pressure function is discontinuous in the phase saturations due to the different properties of the porous matrix on both sides of the discontinuity.

### POROUS MEDIUM DISCONTINUITY SETTINGS

This section is only available if on both sides of the discontinuity a predefined capillary pressure model (**van Genuchten** or **Brooks and Corey**) is active. Select the check box to use automatic settings in this case.

### ENTRY CAPILLARY PRESSURE

This section is only available if automatic settings are not used for the **Porous Medium Discontinuity Settings.**

Specify on which side of the discontinuity the lower permeable medium is located using the settings for the of the **Location of lower permeable medium.**

Specify the **Entry capillary pressure** $p_{\mathrm{ec}}$ (SI unit: Pa) for all phases, except the one computed from the volume constraint. Make sure the values correspond to the settings for the capillary pressure model in the adjacent domain conditions.

### CONSTRAINT SETTINGS

To display this section, click the **Show** 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.*

# The Multiphase Flow in Porous Media Interface

The **Multiphase Flow in Porous Media** interface ( ) combines the **Darcy's Law** interface with the **Phase Transport in Porous Media** interface to model the flow and transport of multiple immiscible phases in a porous medium.

When a predefined **Multiphase Flow in Porous Media** interface is added from **Porous Media and Subsurface Flow** branch ( ) of the **Model Wizard** or **Add Physics** window, **Phase Transport** and **Darcy's Law** interfaces are added to the Model Builder. In addition, the **Multiphysics** node is added, which automatically includes the **Multiphase Flow in Porous Media** multiphysics coupling.

### *On the Constituent Physics Interfaces*

The **Phase Transport in Porous Media** interface is used to simulate the transport of immiscible multiple species in a porous medium and solves for their averaged volume fractions (also called saturations). The interfaces between the different phases are not tracked explicitly, although microscopic interfacial effects are taken into account in the macroscopic equations through the capillary pressure functions.

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

## SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Multiphase Flow in Porous Media**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Phase Transport** and **Darcy's Law** interfaces are added, an empty **Multiphysics** node appears in the model tree. You can choose from the available coupling features but the settings in the constituent interfaces are not modified.

## *Multiphase Flow in Porous Media (Multiphysics Coupling)*

The **Multiphase Flow in Porous Media** multiphysics coupling node () links bidirectionally the **Phase Transport in Porous Media** and **Darcy's Law** interfaces.

### SETTINGS

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

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

The default **Name** (for the first multiphysics coupling feature in the model) is `mfpm1`.

### DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the multiphase flow coupling, or select **All domains** as needed.

When **Multiphase Flow in Porous Media** is added as an effect of adding a Multiphase Flow in Porous Media interface, the selection is the same as for the participating physics interfaces.

Only domains that are active in the physics interfaces selected in the Coupled Interfaces section 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.

# The Fracture Flow Interface

The **Fracture Flow (esff)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to simulate flow along interior boundaries representing fractures within a porous or solid medium. The physics interface uses a variant of Darcy's law and can be used for stationary and time-dependent analysis.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Fluid and Fracture Properties**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, mass sources and conditions on edges or points. You can also right-click **Fracture Flow** to select physics features from the context menu.

### SETTINGS

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

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

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

### 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 (SI unit: $m/s^2$). The default value is taken from the constant `g_const`.

### PHYSICAL MODEL

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

### DEPENDENT VARIABLES

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

### DISCRETIZATION

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

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

## *Domain, Boundary, Edge, Point, and Pair Nodes for the Fracture Flow Interface*

The Fracture Flow Interface has the domain, boundary, edge, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

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

### DOMAIN

- Fluid and Fracture Properties
- Aperture
- Initial Values
- Mass Source
- Storage Model
- Gravity
- Thickness

**Storage Model** and **Mass Source** are described for the Darcy's Law interface and are applied to boundaries instead of domains.

### BOUNDARY CONDITIONS

The boundary conditions for this physics interface are similar to the boundary conditions for The Darcy's Law Interface but are applied to edges in 3D and points in 2D. Edges and points form the "boundaries" of the geometries where the **Fracture Flow** interface is defined, which are faces in 3D and boundaries in 2D.

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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.

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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
- Mass Flux
- Symmetry
- No Flow (the default)
- Atmosphere/Gauge
- Pervious Layer

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 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

---

## *Fluid and Fracture Properties*

The **Fluid and Fracture Properties** node adds Equation 3-6 (excluding any mass sources) on the selected boundary for the pressure and provides an interface for defining the fluid material and its properties, including the effective porosity.

All the nodes are the same as with the Darcy's Law interface (see Fluid and Matrix Properties) except where indicated.

### FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

The default **Density** $\rho$ (SI unit: kg/m$^3$) uses values **From material** based on **Fluid material** selected. For **User defined** enter another value or expression. The default is 0 kg/m$^3$.

The default **Dynamic viscosity** $\mu$ (SI unit: Pa·s) uses values **From material** based on the **Fluid material** selected. For **User defined** enter another value or expression. The default is 0 Pa·s.

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

### FRACTURE PROPERTIES

The default **Porous material** uses the **Boundary material** (the material defined for the fracture domain) for the fracture. Select another material as needed.

#### *Porosity*

The default **Porosity** in the fracture $\varepsilon_f$ (a dimensionless number between 0 and 1) uses values **From material** based on the **Porous material** selected. For **User defined** enter another value or expression. The default is 0.

#### *Permeability Model*

Select a **Permeability model** to specify the capacity of the porous material to transmit flow: **Permeability** to define the permeability of the fracture, **Hydraulic conductivity**, which is a combination of permeability and the dynamic viscosity of water, or **Cubic law** to define the permeability as a function of the fracture's aperture.

- For **Permeability** $\kappa_f$ (SI unit: $m^2$) the default uses values **From material** as defined by the **Porous material** selected. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to enter a tensor value.
- For **Hydraulic conductivity** $K$ (SI unit: m/s) enter a value or expression and select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Anisotropic** to enter a tensor value.
- For **Cubic law** enter a value or expression for the **Roughness factor** $f_f$.

## *Aperture*

The default node to specify the fracture's aperture. Enter a value or expression for the **Aperture** $d_f$ (SI unit: m). The default is 1 mm.

## *Initial Values*

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

### INITIAL VALUES

- Select the **Pressure** (the default) button to enter a value or expression for the initial value of the pressure $p$ (SI unit: Pa). The default is 0 Pa.
- Select **Pressure head** to enter a value or expression for $H_p$ (SI unit: m).
- Select **Hydraulic head** to enter a value or expression for $H$ (SI unit: m).

# The Brinkman Equations Interface

The **Brinkman Equations (br)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. The physics interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. To simplify the equations, select the Stokes-Brinkman flow feature to reduce the dependence on inertial effects when the Reynolds number is significantly less than 1. The physics interface can be used for stationary and time-dependent analyses.

The main node is the Fluid and Matrix Properties feature, which adds the Brinkman equations and provides an interface for defining the fluid material and the porous matrix.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid and Matrix Properties**, **Wall** (the default boundary type, using **No slip** as the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Brinkman Equations** to select physics features from the context menu.

The boundary conditions are essentially the same as for the Laminar Flow interface. Differences exist for the following boundary types: Outlet, Symmetry, Open Boundary, and Boundary Stress where the viscous part of the stress is divided by the porosity to appear as

$$\frac{1}{\varepsilon_\mathrm{p}}\left\{\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}$$

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections such as **Discretization**, **Consistent Stabilization**, and **Inconsistent Stabilization**, and **Advanced Settings** sections, all accessed by clicking the **Show** button ( ) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

## SETTINGS

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

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

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

## PHYSICAL MODEL

This node specifies the properties of the Brinkman Equations interface, which describe the overall type of fluid flow model.

### *Compressibility*

By default the physics interface uses the **Incompressible flow** formulation of the Brinkman equations to model constant density flow. Alternatively, select **Compressible flow (Ma<0.3)** from the **Compressibility** list if there are small variations in the density, typically dependent on the temperature (nonisothermal flow). For compressible flow modeled with the Brinkman Equations interface, the Mach number must be below 0.3.

### *Neglect Inertial Term (Stokes-Brinkman Flow)*

The **Neglect inertial term (Stokes-Brinkman)** check box is selected by default to model flow at very low Reynolds numbers for which the inertial term can be neglected in the Brinkman equations. This results in the linear Stokes-Brinkman equations.

### *Enable porous media domains*

The **Enable porous media domains** check box is selected by default to solve Brinkman equations in porous domains.

### *Reference Pressure Level*

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

## DEPENDENT VARIABLES

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

## ADVANCED SETTINGS

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

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. When selected, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

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- Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface
- Theory for the Brinkman Equations Interface
- Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the *COMSOL Multiphysics Reference Manual*
- Numerical Stability — Stabilization Techniques for Fluid Flow
- Discontinuous Galerkin Formulation

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*Free Convection in Porous Media*: Application Library path **Subsurface_Flow_Module/Heat_Transfer/convection_porous_medium**

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### *Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface*

The Brinkman Equations Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

---

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:

- Fluid and Matrix Properties
- Forchheimer Drag
- Initial Values
- Mass Source
- Volume Force
- Fluid Properties

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

- Flow Continuity
- InletLine Mass Source
- Boundary Stress
- Outlet
- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point ConstraintSymmetry
- Wall

---

! In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

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## *Fluid and Matrix Properties*

The **Fluid and Matrix Properties** node adds the Brinkman equations: Equation 3-20 and Equation 3-21 (excluding any mass sources), and provides an interface for defining the properties of the fluid material and the porous matrix The Forchheimer Drag subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

Both the default **Density** $\rho$ (SI unit: $\mathrm{kg/m^3}$) and **Dynamic viscosity** $\mu$ (SI unit: Pa·s) use values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. In this case, the default is 0 $\mathrm{kg/m^3}$ for the density and 0 Pa·s for the dynamic viscosity. The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. Non-Newtonian fluids have a viscosity that is shear-rate dependent. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions.

#### POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** (the material defined for the domain) for the porous matrix. Select another material as needed.

Both the default **Porosity** $\varepsilon_p$ (a dimensionless number between 0 and 1) and **Permeability** $\kappa$ (SI unit: $m^2$) use values **From material** as defined by the **Porous material** selection. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the characteristics of the permeability, and enter another value or expression. The components of a permeability in the case that it is a tensor ($\kappa_{xx}$, $\kappa_{yy}$, and so on, representing an anisotropic permeability) are available as `br.kappaxx`, `br.kappayy`, and so on (using the default name `br`).

### *Forchheimer Drag*

The **Forchheimer Drag** subnode is available from the context menu (right-click the Fluid and Matrix Properties parent node) or from the **Physics** toolbar, **Attributes** menu. While the drag of the fluid on the porous matrix in the basic Brinkman equations is proportional to the flow velocity, (Darcy's law drag), the Forchheimer drag is proportional to the square of the fluid velocity. The latter term accounts for an inertial turbulent drag effect that comes into play for fast flows through large pores. Adding the Forchheimer term takes into account all drag contributions that the Ergun equation covers.

#### FORCHHEIMER DRAG

Enter a value for the **Forchheimer coefficient** $\beta_F$ (SI unit: $kg/m^4$). The default is $0\ kg/m^4$.

### *Mass Source*

The **Mass Source** node adds a mass source (or mass sink) $Q_{br}$ to the right-hand side of the continuity equation: Equation 3-20. This term accounts for mass deposit and/or mass creation in porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{br} \tag{3-11}$$

#### DOMAIN SELECTION

Only Porous Matrix domains are available.

### MASS SOURCE

Enter a value or expression for the **Source term** $Q_{\mathrm{br}}$ (SI unit: kg/(m$^3$·s)). The default is 0 kg/(m$^3$·s).

## *Volume Force*

Use the **Volume Force** node to specify the force $\mathbf{F}$ on the right-hand side of Equation 3-21. It then acts on each fluid element in the specified domains. A common application is to include gravity effects.

$$\frac{\rho}{\varepsilon_{\mathrm{p}}}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\frac{\mathbf{u}}{\varepsilon_{\mathrm{p}}}\right) = \\ -\nabla p + \nabla\cdot\left[\frac{1}{\varepsilon_{\mathrm{p}}}\left\{\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_{\mathrm{br}}}{\varepsilon_{\mathrm{p}}^2}\right)\mathbf{u} + \mathbf{F} \tag{3-12}$$

### VOLUME FORCE

Enter the components of **Volume force** $\mathbf{F}$ (SI unit: N/m$^3$).

## *Initial Values*

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

### INITIAL VALUES

Enter initial values or expressions for the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and the **Pressure** $p$ (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

## *Fluid Properties*

The **Fluid Properties** node adds the momentum and continuity equations to solve for free flow in 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 $p$+$p_{\mathrm{ref}}$ where $p$ is the dependent pressure variable from the Navier-Stokes equations, and $p_{\mathrm{ref}}$ is from the user input defined at the physics interface level. When $p_{\mathrm{ref}}$ is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, $p_{\mathrm{ref}}$ should be set to 0.

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

### FLUID PROPERTIES

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible.

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

# The Free and Porous Media Flow Interface

The **Free and Porous Media Flow (fp)** interface ( ), found under the **Porous Media and Subsurface Flow** branch ( ) when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow where free flow is connected to porous media. The Free and Porous Media Flow interface is used over at least two different domains: a free channel and a porous medium. The physics interface is well suited for transitions between slow flow in porous media, governed by the Brinkman equations, and fast flow in channels described by the Navier-Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. The physics interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder**— **Fluid Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add a **Fluid and Matrix Properties** node to be used on the domain selection corresponding to the porous media, or add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Free and Porous Media Flow** to select physics features from the context menu.

### SETTINGS

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

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

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

### PHYSICAL MODEL

#### *Compressibility*

By default the physics interface uses the **Incompressible flow** formulation of the Navier-Stokes and Brinkman equations to model constant density flow. If required, select **Compressible flow (Ma<0.3)** from the **Compressibility** list, to account for small variations in the density, typically dependent on the temperature (non-isothermal flow). For compressible flow modeled with this physics interface, the Mach number must be below 0.3.

#### *Neglect Inertial Term*

Select the **Neglect inertial term (Stokes flow)** check box if the inertial forces are small compared to the viscous forces.

#### *Reference Pressure Level*

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

#### *Reference Temperature*

Enter a **Reference temperature** $T_{\mathrm{ref}}$ (SI unit: K). The default value is `293.15[K]`.

### DEPENDENT VARIABLES

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

- Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow Interface
- Theory for the Free and Porous Media Flow Interface

*Forchheimer Flow*: Application Library path **Subsurface_Flow_Module/Fluid_Flow/forchheimer_flow**

## *Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow Interface*

The Free and Porous Media Flow Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

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

- Fluid Properties
- Forchheimer Drag
- Initial Values
- Mass Source
- Fluid and Matrix Properties
- Volume Force
- Wall

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

- No Viscous Stress
- Flow Continuity
- Inlet
- Line Mass Source
- Outlet
- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry

In the *COMSOL Multiphysics Reference Manual* see Table 2-3 for links to common sections and Table 2-4 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

## *Fluid Properties*

Use the **Fluid Properties** node to define the fluid material, density, and dynamic viscosity.

### FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

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

The **Dynamic viscosity** $\mu$ (SI unit: Pa·s) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

## *Fluid and Matrix Properties*

Use the **Fluid and Matrix Properties** node to define which domains contain porous material and to define the porous matrix properties, such as the porosity and permeability in these domains. The Forchheimer Drag subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### DOMAIN SELECTION

Choose domains from the **Selection** list, to solve for porous media flow governed by the Brinkman equations. In the domains not selected, the Free and Porous Media Flow interface solves for laminar flow governed by the Navier-Stokes (or Stokes) equations.

### POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** (the material defined for the domain) for the porous matrix. Select another material as needed.

#### Porosity

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

> ⚠ In this node you specify the porosity $\varepsilon_p$, whereas in other nodes the volume fraction of solid material $\theta_p=1-\varepsilon_p$ is required instead. See Porous Medium in the *Heat Transfer Module User's Guide* for an example.

#### Permeability

The default **Permeability** $\kappa_{br}$ (SI unit: $m^2$) uses values **From material** as defined by the **Porous material** selection. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** from the list and then enter other values or expressions. The components of a permeability in the case that it is a tensor ($\kappa_{xx}$, $\kappa_{yy}$, and so on, representing an anisotropic permeability) are available as `fp.kappaxx`, `fp.kappayy`, and so on (using the default name `fp`). The default is 0 $m^2$.

#### Source Term

Enter a value or expression for an optional mass source (or sink) **Source term** $Q_{br}$ (SI unit: $kg/(m^3 \cdot s)$). This term accounts for mass deposit and mass creation within domains. The physics interface assumes that the mass exchange occurs at zero velocity.

## *Volume Force*

The **Volume Force** node specifies the force $\mathbf{F}$ on the right-hand side of the Navier-Stokes or Brinkman equations, depending on whether the Porous Matrix Properties node is active for the domain. Use it, for example, to incorporate the effects of gravity in a model.

### VOLUME FORCE

Enter the components of the **Volume force** $\mathbf{F}$ (SI unit: $N/m^3$).

## *Forchheimer Drag*

The **Forchheimer Drag** subnode is available from the context menu (right-click the Fluid and Matrix Properties parent node) or from the **Physics** toolbar, **Attributes** menu. It can be used on the domain selection that corresponds to the porous medium. For the Brinkman equations the drag of the fluid on the porous matrix is proportional to the flow velocity, in the same way as for Darcy's law. Add a Forchheimer drag, proportional to the square of the fluid velocity, as needed.

### FORCHHEIMER DRAG

Enter a value for the **Forchheimer coefficient** $\beta_F$ (SI unit: $kg/m^4$).

## *Initial Values*

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

### INITIAL VALUES

Enter initial values or expressions for the **Velocity field** $\mathbf{u}$ (SI unit: m/s) and for the **Pressure** $p$ (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

## *Wall*

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls.

### BOUNDARY CONDITION

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

- No Slip[1]
- Slip
- Leaking Wall

#### *No Slip*

**No slip** is the default boundary condition for a stationary solid wall for laminar flow (and SST, Low Re k-ε, Algebraic yPlus, L-VEL, and Spalart-Allmaras turbulence models). The condition prescribes $\mathbf{u} = 0$; that is, the fluid at the wall is not moving.

#### *Slip*

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

#### *Leaking Wall*

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

### CONSTRAINT SETTINGS

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

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

# 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
- Hydraulic Head, Pressure Head, and Elevation Head
- Average Linear Velocity
- References for the Darcy's Law Interface

## *About Darcy's Law*

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

Darcy's law describes fluid movement through interstices in a porous medium. Because the fluid loses considerable energy to frictional resistance within pores, flow velocities in porous media are very low. The Darcy's Law interface in the Subsurface Flow Module applies to 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:

Darcy's law applies when the gradient in hydraulic potential drives fluid movement in the porous medium. Visualize the hydraulic potential field by considering the difference in both pressure and elevation potential from the start to the end points of the flow line. According to Darcy's law, the net flux across a face of porous surface is

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p + \rho g \nabla D) \tag{3-13}$$

In this equation, **u** is the Darcy velocity or specific discharge vector (SI unit: m/s); $\kappa$ is the permeability of the porous medium (SI unit: $\mathrm{m}^2$); $\mu$ is the fluid's dynamic viscosity (SI unit: Pa·s); $p$ is the fluid's pressure (SI unit: Pa) and $\rho$ is its density (SI unit: $\mathrm{kg/m^3}$); $g$ is the magnitude of gravitational acceleration (SI unit: $\mathrm{m/s^2}$); and $\nabla D$ is a unit vector in the direction over which the gravity acts. Here the permeability, $\kappa$, represents the resistance to flow over a representative volume consisting of many solid grains and pores.

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.

Models can define the capacity to transmit flow using the permeability of the porous medium, $\kappa$, and the viscosity of the fluid, $\mu$, or using the hydraulic conductivity, $K$ (SI unit: m/s).

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

The hydraulic conductivity represents both fluid and solid properties. If the model is defined using the hydraulic conductivity, Equation 3-13 changes to

$$\mathbf{u} = -\frac{\mathbf{K}}{\rho g}(\nabla p + \rho g \nabla D) \tag{3-14}$$

The Kozeny-Carman equation describes the flow through granular soils and packed beds by estimating the permeability of the porous medium from the porosity $\varepsilon$ and average particle diameter $d_\mathrm{p}$

$$\kappa = \frac{d_p^2}{180}\frac{\varepsilon^3}{(1-\varepsilon)^2}$$

If the model is defined using the Kozeny-Carman equation, the expression for Darcy's velocity in Equation 3-13 changes to

$$\mathbf{u} = -\frac{d_p^2}{180\mu}\frac{\varepsilon^3}{(1-\varepsilon)^2}(\nabla p + \rho g \nabla D) \qquad (3\text{-}15)$$

---

The hydraulic conductivity combines properties of both the fluid and porous matrix, while the permeability is a property of the porous matrix only.

---

The hydraulic potential in the equation comes from the pressure, $p$, and gravity, $\rho g D$. COMSOL Multiphysics solves for the pressure, $p$. By default, $g$ is the predefined acceleration of gravity (a physical constant), and $D$ is the vertical coordinate. The choice of $D$ has a significant impact on results and the physics involved. For example, if $D$ is the vertical coordinate $z$ and if the flow is entirely horizontal within the $xy$-plane, then the gradient in $D$ vanishes and the driving force is caused by pressure gradients alone.

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

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_m \qquad (3\text{-}16)$$

In the above equation, $\rho$ is the fluid density (SI unit: $\mathrm{kg/m^3}$), $\varepsilon$ is the porosity, and $Q_m$ is a mass source term (SI unit: $\mathrm{kg/(m^3{\cdot}s)}$). Porosity is defined as the fraction of the control volume that is occupied by pores.

Inserting Darcy's law (Equation 3-13) into the continuity equation produces the generalized governing equation

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot \rho\left[-\frac{\kappa}{\mu}(\nabla p + \rho g \nabla D)\right] = Q_m \qquad (3\text{-}17)$$

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

Expand the time-derivative term in Equation 3-17

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

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

$$\varepsilon\frac{\partial\rho}{\partial t} + \rho\frac{\partial\varepsilon}{\partial t} = \varepsilon\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + \rho\frac{\partial\varepsilon}{\partial p}\frac{\partial p}{\partial t}$$

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

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

Using this relation, the generalized governing equation (Equation 3-17) takes the following form:

$$\rho S\frac{\partial p}{\partial t} + \nabla\cdot\rho\left[-\frac{\kappa}{\mu}(\nabla p + \rho g\nabla D)\right] = Q_{\mathrm{m}} \tag{3-18}$$

In this equation, $S$ is the storage coefficient (SI unit: 1/Pa), which can be interpreted as the weighted compressibility of the porous material and the fluid in the pores. The storage $S$ can be an expression involving results from a solid-deformation equation or an expression involving temperatures and concentrations from other analyses. The Darcy's Law interface implements Equation 3-18 using the Storage Model node, which explicitly includes an option to define $S$ as the *linearized storage* (SI unit: 1/Pa) using the compressibility of fluids and porous solids.

## Hydraulic Head, Pressure Head, and Elevation Head

Hydraulic head, $H$, pressure head, $H_p$, and elevation head, $D$, relate to pressure $p$ as

$$H_p = \frac{p}{\rho g};\quad H = H_p + D \tag{3-19}$$

where $\rho$ is the fluid density, $g$ denotes the acceleration of gravity, and $D$ is the direction over which $g$ acts. When defined as vertical elevation, the horizontal gradients in $D$ equal zero and vertical gradients in $D$ equal one. Choose to specify pressure, hydraulic head, or pressure head on the boundaries of a model, either directly or as part of the pervious layer boundary condition. Also use pressure, hydraulic head, and pressure head during analysis.

Turning off gravity effects sets the elevation $D$ to zero, and the hydraulic head then equals the pressure head.

## *Average Linear Velocity*

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

## *References for the Darcy's Law Interface*

1. J. Bear, *Hydraulics of Groundwater*, McGraw-Hill, 1979.

2. S.E. Ingebritsen and W.E. Sanford, *Groundwater in Geologic Processes*, Cambridge University Press, 1998.

3. N.H. Sleep and K. Fujita, *Principles of Geophysics*, Blackwell Science, 1997.

4. D.L. Turcotte and G. Schubert, *Geodynamics*, Cambridge University Press, 2002.

# 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:

$$\frac{\partial}{\partial t}(\varepsilon_p\rho) + \nabla\cdot(\rho\mathbf{u}) = Q_{\mathrm{br}} \tag{3-20}$$

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) = \\ -\nabla p + \nabla\cdot\left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}\right] - \left(\kappa^{-1}\mu + \frac{Q_{\mathrm{br}}}{\varepsilon_p^2}\right)\mathbf{u} + \mathbf{F} \tag{3-21}$$

In these equations:

- $\mu$ (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- $\mathbf{u}$ (SI unit: m/s) is the velocity vector
- $\rho$ (SI unit: kg/m$^3$) is the density of the fluid
- $p$ (SI unit: Pa) is the pressure
- $\varepsilon_p$ is the porosity
- $\kappa$ (SI unit: m$^2$) is the permeability tensor of the porous medium, and
- $Q_{\mathrm{br}}$ (SI unit: kg/(m$^3$·s)) is a mass source or mass sink

Influence of gravity and other volume forces can be accounted for via the force term $\mathbf{F}$ (SI unit: kg/(m$^2$·s$^2$)).

When the Neglect inertial term (Stokes-Brinkman) check box is selected, the term $(\mathbf{u}\cdot\nabla)(\mathbf{u}/\varepsilon_p)$ on the left-hand side of Equation 3-21 is disabled.

The mass source, $Q_{\mathrm{br}}$, accounts for mass deposit and mass creation within the domains. The mass exchange is assumed to occur at zero velocity.

The Forchheimer drag option, $\beta_F$ (SI unit: kg/m$^4$), adds a viscous force proportional to the square of the fluid velocity, $\mathbf{F}_F = -\beta_F|\mathbf{u}|\mathbf{u}$, to the right-hand side of Equation 3-21.

In case of a flow with variable density, Equation 3-20 and Equation 3-21 must be solved together with the equation of state that relates the density to the temperature and pressure (for instance the ideal gas law).

For incompressible flow, the density stays constant in any fluid particle, which can be expressed as

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

and the continuity equation (Equation 3-20) reduces to

$$\rho\nabla \cdot \mathbf{u} = Q_{\mathrm{br}}$$

## *References for the Brinkman Equations Interface*

1. D. Nield and A. Bejan, *Convection in Porous Media,* 3rd ed., Springer, 2006.

2. M. Le Bars and M.G. Worster, “Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification,” *J. of Fluid Mechanics*, vol. 550, pp. 149–173, 2006.

# Theory for the Free and Porous Media Flow Interface

The Free and Porous Media Flow Interface uses the Navier-Stokes equations to describe the flow in open regions, and the Brinkman equations to describe the flow in porous regions.

The same fields, $\mathbf{u}$ and $p$, are solved for in both the free flow domains and in the porous domains. This means that the pressure in the free fluid and the pressure in the pores is continuous over the interface between a free flow domain and a porous domain. It also means that continuity is enforced between the fluid velocity in the free flow and the Darcy velocity in the porous domain. This treatment is one of several possible models for the physics at the interface. Examples of other models can be found in Ref. 1.

The continuity in $\mathbf{u}$ and $p$ implies a stress discontinuity at the interface between a free-flow domain and a porous domain. The difference corresponds to the stress absorbed by the rigid porous matrix, which is a consequence implicit in the formulations of the Navier-Stokes and Brinkman equations.

## *Reference for the Free and Porous Media Flow Interface*

1. M.L. Bars and M.G. Worster, “Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification,” *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

# Theory for the Fracture Flow Interface

The Fracture Flow Interface theory is described in this section:

- About Fracture Flow
- Equations and Inputs
- Retention and Permeability Relationships

## *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:

$$\mathbf{q}_\mathrm{f} = -\frac{\kappa_\mathrm{f}}{\mu} d_\mathrm{f}(\nabla_\mathrm{T} p + \rho g \nabla_\mathrm{T} D) \tag{3-22}$$

Here, $\mathbf{q}_\mathrm{f}$ is the volume flow rate per unit length in the fracture, $\kappa_\mathrm{f}$ is the fracture's permeability, $\mu$ is the fluid dynamic viscosity, $d_\mathrm{f}$ is the *aperture* or fracture thickness, $\nabla_\mathrm{T}$ 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 $\mathbf{q}_\mathrm{f}$ gives the volume flow rate per unit length of the fracture. The mean fluid velocity within the fracture is $\mathbf{u}_\mathrm{f} = \mathbf{q}_\mathrm{f}/d_\mathrm{f}$.

It is also possible to use the hydraulic conductivity of the fracture, $K_\mathrm{f}$ (SI unit: m/s), to define the capacity to transmit flow instead of using the fracture's permeability $\kappa_\mathrm{f}$ and fluid viscosity $\mu$. These quantities are related by

$$\frac{\kappa_\mathrm{f}}{\mu} = \frac{K_\mathrm{f}}{\rho g}$$

The hydraulic conductivity represents properties of both fluid and porous matrix. If the model is defined using the hydraulic conductivity, Equation 3-22 changes to

$$\mathbf{q}_\mathrm{f} = -\frac{K_\mathrm{f}}{\rho g} d_\mathrm{f}(\nabla_\mathrm{T} p + \rho g \nabla_\mathrm{T} D) \tag{3-23}$$

The Cubic law equation describes the permeability of the fracture from the aperture or fracture's thickness $d_\mathrm{f}$ and the roughness factor $f_\mathrm{f}$

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

If the model is defined using the Cubic law equation, the expression for flow rate per unit length in the fracture in Equation 3-22 changes to

$$\mathbf{q}_\mathrm{f} = -\frac{d_\mathrm{f}^3}{12\mu f_\mathrm{f}}(\nabla_\mathrm{T} p + \rho g \nabla_\mathrm{T} D) \tag{3-24}$$

Together with the material properties, Equation 3-22 above, in combination with the continuity equation integrated over the fracture cross section, produces a single equation for the pressure.

$$d_\mathrm{f}\frac{\partial}{\partial t}(\varepsilon_\mathrm{f}\rho) + \nabla_T \cdot (\rho \mathbf{q}_\mathrm{f}) = d_\mathrm{f} Q_\mathrm{m} \tag{3-25}$$

where $\varepsilon_\mathrm{f}$ is the fracture porosity, and $Q_\mathrm{m}$ is the mass source term (SI unit: kg/(m$^3$·s)). The aperture or fracture thickness $d_\mathrm{f}$ 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 3-25. 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 3-25:

$$\rho S_{\mathrm{f}} d_{\mathrm{f}} \frac{\partial p}{\partial t} - \nabla_T \cdot (\rho \mathbf{q}_{\mathrm{f}}) = d_{\mathrm{f}} Q_m$$

where $S_{\mathrm{f}}$ 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.

# 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.

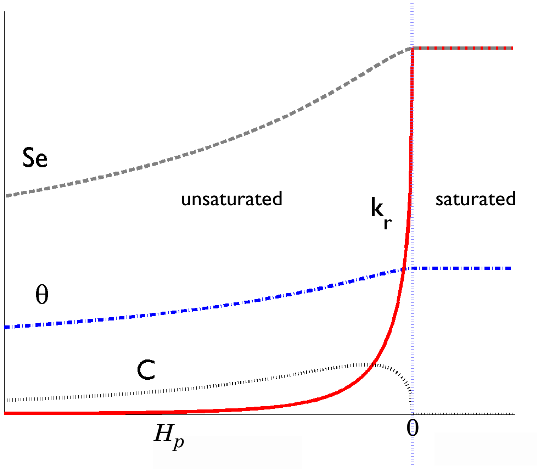

*Figure 3-2: Fluid retention and permeability functions that vary with pressure head, as given by Van Genuchten formulas available in the Richards' Equation interface.*

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):

$$\rho\left(\frac{C_{\mathrm{m}}}{\rho g}+\mathrm{Se}S\right)\frac{\partial p}{\partial t}+\nabla\cdot\rho\left(-\frac{\kappa_{\mathrm{s}}}{\mu}k_{\mathrm{r}}(\nabla p+\rho g\nabla D)\right)=Q_{\mathrm{m}} \qquad (3\text{-}26)$$

where the pressure, $p$, is the dependent variable. In this equation, $C_{\mathrm{m}}$ represents the specific moisture capacity, Se denotes the effective saturation, $S$ is the storage coefficient, $\kappa_{\mathrm{s}}$ gives the hydraulic permeability, $\mu$ is the fluid dynamic viscosity, $k_{\mathrm{r}}$ denotes the relative permeability, $\rho$ is the fluid density, $g$ is acceleration of gravity, $D$ represents the elevation, and $Q_{\mathrm{m}}$ is the fluid source (positive) or sink (negative). Like Darcy's law, COMSOL Multiphysics solves Richards' equation for a dependent variable of pressure but provides features for specifying the values of the hydraulic head or pressure head on the boundaries of a model, either directly or as part of the Pervious Layer boundary condition. Also use the hydraulic head and the pressure head during results evaluation.

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

$$\mathbf{u}=-\frac{\kappa_s}{\mu}k_{\mathrm{r}}(\nabla p+\rho g\nabla D)$$

where $\mathbf{u}$ is the flux 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 volume liquid fraction, $\theta_{\mathrm{s}}$. This interstitial, pore or average linear velocity is $\mathbf{u}_{\mathrm{a}}=\mathbf{u}/\theta_{\mathrm{s}}$.

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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.

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## *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 $\theta$, Se, $C_{\mathrm{m}}$, and $k_{\mathrm{r}}$ 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, $\theta$, ranges from a small residual value $\theta_r$ to the total porosity $\theta_s$. Its value is given in a constitutive relation in the model. The effective saturation, Se, amounts to $\theta$ normalized to a maximum value of 1. The specific moisture capacity, $C_m$, describes the change in $\theta$ as the solution progresses, the slope on a plot of $\theta$ versus pressure (or pressure head). The relative permeability, $k_r$, increases with moisture content and varies from a nominal value to its maximum value 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 $\theta$, Se, $C_m$, and $k_r$:

- The analytic formulas of van Genuchten.
- The analytic formulas of Brooks and Corey.
- A 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.

The van Genuchten equations define saturation when the fluid pressure is atmospheric (that is, $H_p = 0$). These equations are

$$\theta = \begin{cases} \theta_r + \mathrm{Se}(\theta_s - \theta_r) & H_p < 0 \\ \theta_s & H_p \geq 0 \end{cases}$$

$$\mathrm{Se} = \begin{cases} \dfrac{1}{[1 + |\alpha H_p|^n]^m} & H_p < 0 \\ 1 & H_p \geq 0 \end{cases}$$

$$C_m = \begin{cases} \dfrac{\alpha m}{1 - m}(\theta_s - \theta_r)\mathrm{Se}^{\frac{1}{m}}\left(1 - \mathrm{Se}^{\frac{1}{m}}\right)^m & H_p < 0 \\ 0 & H_p \geq 0 \end{cases} \tag{3-27}$$

$$k_r = \begin{cases} \mathrm{Se}^l\left[1 - \left(1 - \mathrm{Se}^{\frac{1}{m}}\right)^m\right]^2 & H_p < 0 \\ 1 & H_p \geq 0 \end{cases}$$

here, the constitutive parameter $m$ is equal to $1 - 1/n$. 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

$$\theta = \begin{cases} \theta_r + \mathrm{Se}(\theta_s - \theta_r) & H_p < -\dfrac{1}{\alpha} \\ \theta_s & -\dfrac{1}{\alpha} \le H_p \end{cases}$$

$$\mathrm{Se} = \begin{cases} \dfrac{1}{\left|\alpha H_p\right|^n} & H_p < -\dfrac{1}{\alpha} \\ 1 & -\dfrac{1}{\alpha} \le H_p \end{cases}$$

$$C_m = \begin{cases} \dfrac{-n}{H_p}(\theta_s - \theta_r)\dfrac{1}{\left|\alpha H_p\right|^n} & H_p < -\dfrac{1}{\alpha} \\ 0 & -\dfrac{1}{\alpha} \le H_p \end{cases} \tag{3-28}$$

$$k_r = \begin{cases} \mathrm{Se}^{\frac{2}{n} + l + 2} & H_p < -\dfrac{1}{\alpha} \\ 1 & -\dfrac{1}{\alpha} \le H_p \end{cases}$$

Here, the constitutive parameter $m$ is equal to $1 - 1/n$. COMSOL Multiphysics also provides user-defined options for those who want to incorporate experimental data or arbitrary expressions to define these relationships.

## *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.

# Theory for the Two-Phase Darcy's Law Interface

## *Darcy's Law*

Darcy's law states that the velocity field is determined by the pressure gradient, the fluid viscosity, and the permeability of the porous medium. According to Darcy's law, the velocity field is given by

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p \tag{3-29}$$

In this equation:

- $\mathbf{u}$ (SI unit: m/s) is the Darcy velocity vector
- $\kappa$ (SI unit: $\mathrm{m}^2$) is the permeability of the porous medium
- $\mu$ (SI unit: Pa·s) is the fluid's dynamic viscosity, and
- $p$ (SI unit: Pa) is the fluid's pressure

The permeability, κ, represents the resistance to flow over a representative volume consisting of solid grains and pores.

The Two-Phase Darcy's Law interface combines Darcy's law (Equation 3-13) with the continuity equation for the average density ρ

$$\frac{\partial}{\partial t}(\rho\varepsilon_{\mathrm{p}}) + \nabla\cdot(\rho\mathbf{u}) = 0 \tag{3-30}$$

here, $\varepsilon_{\mathrm{p}}$ is the porosity, defined as the fraction of the control volume that is occupied by pores. Inserting Darcy's law (Equation 3-13) into the continuity equation (Equation 3-30) produces the governing equation

$$\frac{\partial}{\partial t}(\rho\varepsilon_{\mathrm{p}}) + \nabla\cdot\rho\left[-\frac{\kappa}{\mu}\nabla p\right] = 0 \tag{3-31}$$

In the presence of two miscible fluid phases, the average density ρ and average viscosity μ depend on the composition of the mixture (Ref. 6). In the Two-Phase Darcy's Law interface these dependencies are given by

$$1 = s_1 + s_2 \tag{3-32}$$

$$\rho = s_1\rho_1 + s_2\rho_2 \tag{3-33}$$

$$\frac{1}{\mu} = s_1\frac{\kappa_{r1}}{\mu_1} + s_2\frac{\kappa_{r2}}{\mu_2} \tag{3-34}$$

here, $s_1$ and $s_2$ represent the saturation of each phase, $\rho_1$ and $\rho_2$ the densities, and $\kappa_{r1}$ and $\kappa_{r2}$ the relative permeabilities. When either of the fluids is compressible, its density can be related to the pressure (for instance using the ideal gas law).

## *Capillary Pressure*

Beside the continuity equation for the mixture (Equation 3-17), the Two-Phase Darcy's Law interface also solves the transport equation for the fluid content of one of the phases, $c_1 = s_1\rho_1$

$$\frac{\partial}{\partial t}(\varepsilon_p c_1) + \nabla \cdot (c_1\mathbf{u}) = \nabla \cdot D_c \nabla c_1 \tag{3-35}$$

here, $D_c$ (SI unit: $m^2/s$) is the capillary diffusion coefficient, which can be directly specified, or it can be derived from a capillary pressure expression. Normally, the fluid content $c_1$ will be the concentration of the wetting phase.

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

$$D_c = \frac{\kappa_{r1}}{\mu_1}\kappa(s_1 - 1)\frac{\partial p_c}{\partial s_1} \tag{3-36}$$

The capillary pressure is defined as the pressure difference between the phases, and it can be defined as a function of saturation, $p_c(s_1)$. The capillary pressure can be a user defined expression, or it can be derived from van Genuchten (Ref. 7) or Brooks and Corey (Ref. 8) models.

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

$$p_c = p_{ec}\left(\frac{1}{s_1^{1/m}} - 1\right)^{1-m} \tag{3-37}$$

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

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

$$p_c = p_{ec}\frac{1}{s_1^{1/\lambda}} \tag{3-38}$$

where λ is the pore distribution index.

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

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

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

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

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

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

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

where λ is again the pore distribution index.

## *References for the Two-Phase Darcy's Law interface*

6. Z. Chen, G. Huan, and Y. Ma, *Computational Methods for Multiphase Flows in Porous Media*. Philadelphia: Society for Industrial and Applied Mathematics, 2006.

7. M.Th. van Genuchten, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," *Soil Sci. Soc. Am. J.*, vol. 44, 1980.

8. R.H. Brooks and A.T. Corey, "Properties of Porous Media Affecting Fluid Flow," *J. Irrig. Drainage Div., ASCE Proc.*, vol. 72 (IR2), 1966.

# Theory for the Phase Transport Interface

The **Phase Transport** interface provides a predefined modeling environment for studying the transport of multiple immiscible fluid, gas, or (dispersed) solid phases either in free flow or in flow through a porous medium. This interface solves for the averaged volume fractions (also called saturations in a porous medium) of the phases, and does not track the interfaces between the different phases. The **Phase Transport** interface is based on the macroscopic mass conservation equations of each phase. In a porous medium the effects of the microscopic (or pore scale) interfaces between the phases can be taken into account via the capillary pressure functions.

## *Phase Transport in Free Flow*

Suppose the fluid consists of a mixture of $i = 1, \ldots, N$ immiscible phases. The following mass conservation equation describes the transport for an individual phase:

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) = Q_i \qquad (3\text{-}39)$$

where $\rho_i$ denotes the density (SI unit: kg/m$^3$), $s_i$ denotes the volume fraction (dimensionless), and $\mathbf{u}_i$ denotes the velocity vector (SI unit: m/s) of phase $i$. In addition, the term $Q_i$ denotes a mass source for phase $i$ (SI unit: kg/(m$^3$·s)). It is assumed that the sum of the volume fractions of the phases equals 1:

$$\sum_{i=1}^{N} s_i = 1 \qquad (3\text{-}40)$$

This means that $N - 1$ phase volume fractions are independent and are possible to solve for using Equation 3-39. The volume constraint Equation 3-40 is used to reduce the number of dependent variables: one volume fraction, let us say of phase $i_c$ (to be specified in the main node of the **Phase Transport** interface), is expressed using the other volume fractions:

$$s_{i_c} = 1 - \left( \sum_{i=1, i \neq i_c}^{N} s_i \right) \qquad (3\text{-}41)$$

### Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The **Phase Transport** interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis. In this case it adds a diffusion term proportional to the turbulent kinematic viscosity to the phase transport Equation 3-39, which then becomes

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) - \nabla \cdot \left(\rho_i \frac{\nu_\mathrm{T}}{\mathrm{Sc}_\mathrm{T}} \nabla s_i\right) = \boldsymbol{Q}_i \qquad \text{for} \quad i \neq i_c \tag{3-42}$$

### Phase Transport in Porous Media

In a porous domain, the mass conservation equation for each phase is given by:

$$\frac{\partial}{\partial t}(\varepsilon_\mathrm{p} \rho_i s_i) + \nabla \cdot (\rho_i \mathbf{u}_i) = \boldsymbol{Q}_i \tag{3-43}$$

Here $\varepsilon_\mathrm{p}$ (dimensionless) is the porosity, and the vector $\mathbf{u}_i$ should now be interpreted as the volumetric flux of phase $i$ (SI unit $\mathrm{m}^3/(\mathrm{m}^2 \cdot \mathrm{s})$ or m/s). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_i = -\frac{\kappa_{\mathrm{r}i}}{\mu_i} \kappa (\nabla p_i - \rho_i \mathbf{g}) \tag{3-44}$$

where $\kappa$ denotes the permeability (SI unit: $\mathrm{m}^2$) of the porous medium, $\mathbf{g}$ the gravitational acceleration vector (SI unit $\mathrm{m/s}^2$), and $\mu_i$ the dynamic viscosity (SI unit: kg/(m·s)), $p_i$ the pressure field (SI unit: Pa), and $\kappa_{\mathrm{r}i}$ the relative permeability (dimensionless) of phase $i$, respectively.

One phase pressure can be chosen independently, which in the **Phase Transport in Porous Media** interface is chosen to be the phase pressure, $p_{i_c}$, of the phase computed from the volume constraint, and the other phase pressures are defined by the following $N - 1$ capillary pressure relations:

$$p_i = p_{i_c} + p_{\mathrm{c}_i}(s_1, \ldots, s_N) \qquad \text{for} \quad i \neq i_c \tag{3-45}$$

Substituting Equation 3-44 into Equation 3-43, and using the volume constraint in Equation 3-40, we arrive at the following $N-1$ equations for the phase volume fractions $s_i$, $(i \neq i_c)$ that are solved in the **Phase Transport in Porous Media** interface:

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p}}\rho_i s_i) - \nabla\cdot\left(\rho_i\kappa_{\mathrm{r}i}\frac{\kappa}{\mu_i}(\nabla(p_{i_c}+p_{\mathrm{c}_i})-\rho_i\mathbf{g})\right) = \mathbf{Q}_i \qquad \text{for} \quad i \neq i_c \tag{3-46}$$

The remaining volume fraction is computed from

$$s_{i_c} = 1 - \left(\sum_{i=1,\, i\neq i_c}^{N} s_i\right) \tag{3-47}$$

## *Predefined Capillary Pressure and Relative Permeability Models*

The capillary pressure functions $p_{\mathrm{c}_i}$ can be supplied as user defined expressions, or, in case there are only two phases present in the **Phase Transport in Porous Media** interface, the capillary pressure function can be derived from van Genuchten (Ref. 7) or Brooks and Corey (Ref. 8) models. When either of these predefined models is used, the user has to specify which phase is the wetting phase. If the wetting phase is the same as the phase computed from the volume constraint, then

$$p_i = p_{i_c} + p_{\mathrm{c}} \qquad \text{for} \quad i \neq i_c \tag{3-48}$$

otherwise

$$p_i = p_{i_c} - p_{\mathrm{c}} \qquad \text{for} \quad i \neq i_c \tag{3-49}$$

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

$$p_{\mathrm{c}} = p_{\mathrm{ec}}\left(\frac{1}{(\overline{s}_{\mathrm{w}})^{1/m_{\mathrm{vG}}}} - 1\right)^{1-m_{\mathrm{vG}}} \tag{3-50}$$

where $p_{\mathrm{ec}}$ is the entry capillary pressure and $m_{\mathrm{vG}}$ is a constitutive constant, and where $\overline{s}_{\mathrm{w}}$ denotes the effective saturation of the wetting phase. The effective saturation of each phase is defined as

$$\overline{s}_i = (s_i - s_{\mathrm{r}i})/\left(1 - \sum_{j=1}^{N} s_{\mathrm{r}j}\right) \tag{3-51}$$

where $s_{rj}$ denotes the residual saturation of phase $j$. For the Brooks and Corey model, the capillary pressure curve depends on saturation as

$$p_{\mathrm{c}} = p_{\mathrm{ec}}\frac{1}{(\overline{s}_{\mathrm{w}})^{1/\lambda_{\mathrm{p}}}} \tag{3-52}$$

where $\lambda_{\mathrm{p}}$ is the pore distribution index.

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

$$\kappa_{\mathrm{r}s_{\mathrm{w}}} = (\overline{s}_{\mathrm{w}})^{l_{\mathrm{vG}}}\left(1-(1-(\overline{s}_{\mathrm{w}})^{1/m_{\mathrm{vG}}})^{m_{\mathrm{vG}}}\right)^{2} \tag{3-53}$$

$$\kappa_{\mathrm{r}s_{\mathrm{n}}} = (\overline{s}_{\mathrm{n}})^{l_{\mathrm{vG}}}(1-(1-\overline{s}_{\mathrm{n}})^{1/m_{\mathrm{vG}}})^{2m_{\mathrm{vG}}} \tag{3-54}$$

where $m_{\mathrm{vG}}$ and $l_{\mathrm{vG}}$ are constitutive constants, and where $s_{\mathrm{n}}$ denotes the volume fraction of the nonwetting phase. For the Brooks and Corey model, the relative permeabilities are given by

$$\kappa_{\mathrm{r}s_{\mathrm{w}}} = (\overline{s}_{\mathrm{w}})^{(3+2/\lambda_{\mathrm{p}})} \tag{3-55}$$

$$\kappa_{\mathrm{r}s_{\mathrm{n}}} = \overline{s}_{\mathrm{n}}^{2}(1-(1-\overline{s}_{\mathrm{n}})^{(1+2/\lambda_{\mathrm{p}})}) \tag{3-56}$$

where $\lambda_{\mathrm{p}}$ is again the pore distribution index.

## *Porous Medium Discontinuity Boundary Condition*

Over a boundary between a more permeable and a less permeable porous domain the macroscopic saturation of the different phases is often discontinuous. The **Porous Medium Discontinuity** boundary condition implements the following condition on such an interior boundary:

$$p_{\mathrm{c}_i}^{l}(s_i^{l}) = \begin{cases} p_{\mathrm{ec},\,i}^{l} & \text{if} \quad p_{\mathrm{c}_i}^{h}(s_i^{h}) \le p_{\mathrm{ec},\,i}^{l} \\ p_{\mathrm{c}_i}^{h}(s_i^{h}) & \text{if} \quad p_{\mathrm{c}_i}^{h}(s_i^{h}) > p_{\mathrm{ec},\,i}^{l} \end{cases} \qquad \text{for} \quad i \ne i_c \tag{3-57}$$

where the superscript $l$ is used to indicate the saturation and capillary pressure on the low permeable side of the boundary and the superscript $h$ indicates the high permeable side. The first case implements the condition that if the capillary pressure on the more permeable side is lower than the entry capillary pressure on the less permeable side, then the saturation of phase $i$ on the less permeable side equals 0 (or the residual saturation), and the second case implements the condition that if the capillary pressure on the more permeable side is higher than the entry capillary pressure on the less permeable side, the phase $i$ is present on both sides of the interface, and that in this case the capillary pressure is continuous over the interface.

The additional conditions are continuity of the fluxes for all phases and continuity of the pressure of the phase $i_c$ computed from the volume constraint. Note that this last condition assumes that this phase is present on both sides of the porous medium discontinuity boundary condition. In addition this boundary condition assumes that the phase $i_c$ computed from the volume constraint is the wetting phase and it is necessary that the settings for the van Genuchten or Brooks and Corey capillary pressure model match this assumption.

## *References*

9. M.Th. van Genuchten, “A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils,” *Soil Sci. Soc. Am. J.*, vol. 44, 1980.

10. R.H. Brooks and A.T. Corey, “Properties of Porous Media Affecting Fluid Flow,” J. Irrig. Drainage Div., *ASCE Proc.*, vol. 72 (IR2), 1966.

# Theory for the Multiphase Flow in Porous Media Interface

The model equations that are solved in the **Multiphase Flow in Porous Media** interface are based on the mass conservation of each phase and on an extended Darcy's law. The mass conservation equation for each phase is given by

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p}}\rho_i s_i) + \nabla\cdot(\rho_i \mathbf{u}_i) = Q_i \tag{3-58}$$

where $\varepsilon_{\mathrm{p}}$ (dimensionless) is the porosity, and the vector $\mathbf{u}_i$ should be interpreted as the volumetric flux of phase $i$ (SI unit $\mathrm{m}^3/(\mathrm{m}^2\cdot\mathrm{s})$ or m/s). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_i = -\frac{\kappa_{\mathrm{r}i}}{\mu_i}\kappa(\nabla p_i - \rho_i \mathbf{g}) \tag{3-59}$$

where $\kappa$ denotes the permeability (SI unit: $\mathrm{m}^2$) of the porous medium, $\mathbf{g}$ the gravitational acceleration vector (SI unit $\mathrm{m/s}^2$), and $\mu_i$ the dynamic viscosity (SI unit: kg/(m·s)), $p_i$ the pressure field (SI unit: Pa), and $\kappa_{\mathrm{r}i}$ the relative permeability (dimensionless) of phase $i$, respectively. The phase pressures $p_i$ are related through the capillary pressure functions $p_{\mathrm{c}_{ij}}$:

$$p_i - p_j = p_{\mathrm{c}_{ij}}(s_1, \ldots, s_N) \qquad i \neq j \tag{3-60}$$

One phase pressure can be chosen independently so that $N-1$ capillary pressure relations are needed to define the other phase pressures. In addition it is assume that all phases together fill the pore space completely, so that we have

$$\sum_{i=1}^{N} s_i = 1 \tag{3-61}$$

## *Pressure-Saturation Formulation*

The algebraic relations in Equation 3-60 and Equation 3-61 allow for a reduction of the number of dependent variables. An often used way is to eliminate $N-1$ phase pressures and one of the saturations. This results in a so-called pressure-saturation formulation (Ref. 3). The procedure in the **Multiphase Flow in Porous Media** interface is to pick one of the phases, let us say phase $i_c$, then express the volume fraction, $s_{i_c}$, of this phase in terms of the volume fractions of the other phases and in addition to use the pressure, $p_{i_c}$, of this phase to define the other phase pressures:

$$s_{i_c} = 1 - \left( \sum_{i = 1, i \neq i_c}^{N} s_i \right) \tag{3-62}$$

$$p_i = p_{i_c} + p_{c_{ij}}(s_1, \ldots, s_N) \qquad \text{for} \quad i \neq i_c \tag{3-63}$$

The equations for the volume fractions $s_i$, $(i \neq i_c)$ are given by Equation 3-58 and Equation 3-59. To arrive at an equation for $p_i$, the conservation equations of all phases are summed. This results in

$$\frac{\partial}{\partial t}\left( \varepsilon_{\mathrm{p}} \sum_{i = 1}^{N} \rho_i s_i \right) + \nabla \cdot \left( \sum_{i = 1}^{N} \rho_i \mathbf{u}_i \right) = Q_{\mathrm{tot}} \tag{3-64}$$

where the total mass source $Q_{\mathrm{tot}}$ is given by

$$Q_{\mathrm{tot}} = \sum_{i = 1}^{N} Q_i \tag{3-65}$$

The equations for the volume fractions $s_i$ are solved in the **Phase Transport in Porous Media** interface (see Equation 3-43 and Equation 3-44). The Equation 3-64 for the pressure field $p_{i_c}$, needed as an input to the **Phase Transport in Porous Media** interface, is solved for in the **Darcy's Law** interface: the **Multiphase Flow in Porous Media** multiphysics coupling interface replaces the equation

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p}} \rho_{i_c}) + \nabla \cdot (\rho_{i_c} \mathbf{u}_{\mathrm{d}}) = Q_{\mathrm{m}} \quad \text{where} \quad \mathbf{u}_{\mathrm{d}} = -\frac{1}{\mu_{i_c}} \kappa (\nabla p_{i_c} - \rho_{i_c} \mathbf{g}) \tag{3-66}$$

which is originally implemented in the **Darcy's Law** interface, with Equation 3-64 by adding the following terms to the left-hand side of Equation 3-66:

$$\frac{\partial}{\partial t}\left( \varepsilon_{\mathrm{p}} \sum_{i = 1}^{N} \rho_i s_i - \varepsilon_{\mathrm{p}} \rho_{i_c} \right) + \nabla \cdot \left( \sum_{i = 1}^{N} \rho_i \mathbf{u}_i - (\rho_{i_c} \mathbf{u}_{\mathrm{d}}) \right) \tag{3-67}$$

and by it setting the right-hand side $Q_{\mathrm{m}}$ to be equal to $Q_{\mathrm{tot}}$.

Furthermore, the **Multiphase Flow in Porous Media** multiphysics coupling interface couples the user inputs for the porosity and permeability of the porous matrix in the **Darcy's Law** interface to the corresponding user input fields in the **Phase and Porous Media Transport Properties** feature, and couples the pressure field computed for in the **Darcy's Law** interface to the user input field for the pressure of the phase computed from the volume constraint. In the other direction, the multiphysics coupling node provides the density and viscosity of the phase computed from the volume constraint 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, $Q_{\mathrm{tot}}$, equals zero. This implies

$$Q_{i_c} = -\sum_{i=1,\, i \neq i_c}^{N} Q_i \tag{3-68}$$

However, when mass is transfered 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 3-64 for $p_{i_c}$.

### Boundary Conditions

When supplying boundary conditions for the coupled **Phase Transport in Porous Media** and **Darcy's Law** interfaces, bear in mind that the **Pressure** boundary condition in the **Darcy's Law** interface affects the pressure of the phase from the volume constraint, $p_{i_c}$. If the pressure of another phase needs to supplied, take into account the capillary pressure.

Since the coupled **Darcy's Law** interface uses the conservation equation for the total mass (Equation 3-64) to solve for $p_{i_c}$, the **Mass Flux** boundary condition in the **Darcy's Law** interface should be used to prescribe the mass flux of all phases together.

If the mass flux of the phase computed from the volume constraint needs to be prescribed at a boundary, and the total mass flux is not known a priori, it might be necessary to compute for the total mass flux in the form of a Lagrange multiplier by using the weak constraint formulation for the pressure boundary condition in the **Darcy's Law** interface.

## *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.

# 4

# 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 Transport of Diluted Species Interface

The **Transport of Diluted Species (tds)** interface ( ), found under the **Chemical Species Transport** branch ( ), is used to calculate the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid, or solid can be handled with this interface. The driving forces for transport can be diffusion by Fick's law, convection when coupled to a flow field, and migration, when coupled to an electric field.

The interface supports simulation of transport by convection and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, $c$. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, $c_i$, of each species $i$.

### SETTINGS

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

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

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

### DOMAIN SELECTION

If any part of the model geometry should not partake in the mass transfer model, remove that part from the selection list.

### 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 available in all products. For details see http://www.comsol.com/products/specifications/.

- By default, the **Convection** check box is selected. Clear the check box to disable convective transport.
- Select the **Migration in electric field** check box to activate transport of ionic species in an electric field. See further the theory section Adding Transport Through Migration.

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! Transport of ionic species in an electric field is available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

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### *Mass Transport in Porous Media*

The **Mass transport in porous media** check box activates functionality specific to species transport in porous media. When selected, the following transport mechanisms are available:

- Select the **Dispersion in porous media** check box to activate the dispersion mechanism in porous media. See further Dispersion in the theory chapter.
- Select the **Volatilization in partially saturated porous media** check box to model volatilization in partially saturated domains. See further Theory for the Transport of Diluted Species Interface.

The following features are also enabled when selecting the **Mass transport in porous media** check box:

- Adsorption
- Fracture
- Partially Saturated Porous Media
- Porous Media Transport Properties

### CONSISTENT STABILIZATION

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

- When the **Crosswind diffusion** check box is selected, a weak term that reduces spurious oscillations is added to the transport equation. The resulting equation system is always nonlinear. There are two options for the **Crosswind diffusion type**:
    - **Do Carmo and Galeão** — the default option. This type of crosswind diffusion reduces undershoots and overshoots to a minimum but can in rare cases give equation systems that are difficult to fully converge.
    - **Codina**. This option is less diffusive compared to the Do Carmo and Galeão option but can result in more undershoots and overshoots. It is also less effective for anisotropic meshes. The Codina option activates a text field for the **Lower gradient limit** $g_{\mathrm{lim}}$. It defaults to `0.1[mol/m^3)/tds.helem`, where `tds.helem` is the local element size.
- For both consistent stabilization methods, select an **Equation residual**. **Approximate residual** is the default and means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is computationally faster. If required, select **Full residual** instead.

### INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**. By default, the **Isotropic diffusion** check box is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for underresolved problems.

### ADVANCED SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Normally these settings do not need to be changed. Select a **Convective term**—**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 see all settings available in this section, click the **Show** button ( ) and select **Advanced Physics Options**.

The **Compute boundary fluxes** check box is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option is checked, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the check box is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

The flux variables affected in the interface are:

- `ndflux_c` (where *c* is the dependent variable for the concentration). This is the normal diffusive flux and corresponds to the boundary flux when diffusion is the only contribution to the flux term.
- `ntflux_c` (where *c* is the dependent variable for the concentration). This is the normal total flux and corresponds to the boundary flux plus additional transport terms, for example, the convective flux when you use the nonconservative form.

Also the **Apply smoothing to boundary fluxes** check box is available if the previous check box is checked. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the *COMSOL Multiphysics Reference Manual*.

The **Value type when using splitting of complex variables** setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

### DEPENDENT VARIABLES

The dependent variable name is the **Concentration** *c* by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the **Number of species**. Use the **Add concentration** ( + ) and **Remove concentration** ( ☒ ) buttons as needed.

#### FURTHER READING

- Theory for the Transport of Diluted Species Interface
- Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*.
- In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

- *Effective Diffusivity in Porous Materials*: Application Library path **COMSOL_Multiphysics/Diffusion/effective_diffusivity**
- *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 Media Transport Properties node is added by default. The interface includes reaction rate expressions and solute sources for modeling of species transport and reaction in porous media.

This interface is dedicated to modeling transport in porous media, including immobile and mobile phases, where the chemical species may be subjected to diffusion, convection, migration, dispersion, adsorption, and volatilization in porous media. It supports cases where either the solid phase substrate is exclusively immobile, or when a gas-filling medium is also assumed to be immobile.

It applies to one or more diluted species or solutes that move primarily within a fluid that fills (saturated) or partially fills (unsaturated) the voids in a solid porous medium. The pore space not filled with fluid contains an immobile gas phase. Models including a combination of porous media types can be studied.

The main feature nodes are the **Porous Media Transport Properties** and **Partially Saturated Porous Media** nodes, which add the equations for the species concentrations and provide an interface for defining the properties of the porous media, as well as additional properties governing adsorption, volatilization, dispersion and diffusion, migration, and the velocity field to model convection.

The physics interface can be used for stationary and time-dependent analysis.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Porous Media Transport Properties**, **No Flux** (the default boundary condition), and **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

- Theory for the Transport of Diluted Species Interface
- Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

- *Variably Saturated Flow and Transport — Sorbing Solute*: Application Library path **Subsurface_Flow_Module/Solute_Transport/sorbing_solute**

  Web link: http://www.comsol.com/model/variably-saturated-flow-and-transport-sorbing-solute-490

## *Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface*

The Transport of Diluted Species Interface has the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar

(Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

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

- Adsorption
- Concentration
- Electrode Surface Coupling
- Equilibrium Reaction
- Fast Irreversible Surface Reaction
- Flux
- Flux Discontinuity
- Fracture
- Inflow
- Initial Values
- Line Mass Source
- Mass-Based Concentrations
- No Flux
- Open Boundary
- Outflow
- Partially Saturated Porous Media
- Partition Condition
- Periodic Condition
- Point Mass Source
- Porous Electrode Coupling
- Porous Media Transport Properties
- Reaction Coefficients
- Reactions
- Reactive Pellet Bed
- Species Source
- Surface Reactions
- Surface Equilibrium Reaction
- Symmetry
- Thin Diffusion Barrier
- Thin Impermeable Barrier
- Transport Properties
- Turbulent Mixing
- Volatilization

Some features require certain add-on modules. See details http://www.comsol.com/products/specifications/

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

In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

## *Transport Properties*

The settings in this node are dependent on the check boxes selected under Transport Mechanisms on the Settings window for the Transport of Diluted Species interface. It includes only the sections required by the activated transport mechanisms. It has all the equations defining transport of diluted species as well as inputs for the material properties.

When the **Convection** check box is selected, the Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu.

### MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

### CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

### DIFFUSION

Select an option from the **Material** list. This selection list can only be used if a material has been added in the Materials node and if that material has a diffusion coefficient defined. Else, you need to type in the diffusivity in the **User Defined** edit field.

Enter the **Diffusion coefficient** $D_c$ for each species. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: http://www.comsol.com/products/specifications/.

### MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

- Enter a value or expression for the **Electric potential** $V$, which is **User defined**; this input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has also been added to the model.
- Select the electric potential defined or solved by Electrochemistry interface that has been added to the component.

By default the **Mobility** is set to be calculated based on the species diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, and under **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** — and type in the value of expression of the mobility $u_{m,c}$.

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

#### EXAMPLE MODELS

- *Separation Through Dialysis*: Application Library path **Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis**

  Web link: http://www.comsol.com/model/separation-through-dialysis-258

- *Transport in an Electrokinetic Valve*: Application Library path **Microfluidics_Module/Fluid_Flow/electrokinetic_valve**

  Web link: http://www.comsol.com/model/electrokinetic-valve-603

## *Turbulent Mixing*

Use this node to account for the turbulent mixing of the chemical species caused by the eddy diffusivity. This node should typically be used when the specified velocity field corresponds to a RANS solution.

! This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

The subnode can added from the context menu (right-click the Transport Properties parent node), as well as from the **Physics** toolbar, **Attributes** menu, provided that **Convection** is selected as a transport mechanism.

#### TURBULENT MIXING PARAMETERS

Some physics interfaces provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** $\nu_T$ list. The list always contains the **User defined** option where any value or expression can be entered.

The default **Turbulent Schmidt number** $Sc_T$ is 0.71 (dimensionless).

#### FURTHER READING

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

## *Initial Values*

The **Initial Values** node specifies the initial values for the concentration of each species. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

### DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

### INITIAL VALUES

Enter a value or expression for the initial value of the **Concentration** or concentrations, $c_i$. This also serves as a starting guess for stationary problems.

## *Mass-Based Concentrations*

Use the **Mass-Based Concentrations** node to add postprocessing variables for mass-based concentrations (SI unit: $kg/m^3$) and mass fractions (dimensionless) for all species.

### MIXTURE PROPERTIES

The default **Solvent density** $\rho_{solvent}$ is taken **From material**. For **User defined,** enter a value or expression manually. Define the **Molar mass** of each species, which is needed to calculate the mass-based concentration.

## *Reactions*

Use the **Reactions** node to account for the consumption or production of species through chemical reactions. Define the rate expressions as required.

### DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

### REACTION RATES

Add a rate expression $R$ (SI unit: $mol/(m^3{\cdot}s)$) for species $i$. Enter a value or expression in the field. Note that if you have the *Chemistry* interface available, provided with the

*Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down menu. For an example, see the application *Fine Chemical Production in a Plate Reactor* as linked below.

### REACTING VOLUME

This section is only available when the Mass Transport in Porous Media property is available and selected. See http://www.comsol.com/products/specifications/ for more details on availability.

When specifying reaction rates for a species in porous media, the specified reaction rate may have the basis of the total volume, the pore volume, or the volume of a particular phase.

- For **Total volume**, the reaction expressions in mol/($m^3$·s) are specified per unit volume of the model domain (multiplied by unity).
- For **Pore volume**, the reaction expressions in mol/($m^3$·s) are specified per unit volume of total pore space. The reaction expressions will be multiplied by the domain porosity, $\varepsilon_p$. ($\varepsilon_p$ equals unity for nonporous domains.)
- For **Liquid phase**, the reaction expressions in mol/($m^3$·s) are specified per unit volume of liquid in the pore space. The expressions will be multiplied by the liquid volume fraction $\theta$. ($\theta$ equals $\varepsilon_p$ for Saturated Porous Media domains).
- For **Gas phase**, the expressions are multiplied by the gas volume fraction $a_v = \varepsilon_p - \theta$. $a_v$ equals 0 for Saturated Porous Media domains.

### FURTHER READING

See the theory chapter on chemical species transport, starting with the section *Mass Balance Equation*.

---

- *Fine Chemical Production in a Plate Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/plate_reactor**

  Web link: http://www.comsol.com/model/fine-chemical-production-in-a-plate-reactor-8589

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### *No Flux*

This node is the default boundary condition on exterior boundaries. It should be used on boundaries across which there is no mass flux, typically exterior solid walls where no surface reactions occur. The condition applied for each species corresponds to

$$-\mathbf{n}\cdot\mathbf{J}_i = 0$$

### *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 $c_{0,\mathrm{c}}$ (SI unit: $\mathrm{mol/m^3}$), enter a value or expression.

#### BOUNDARY CONDITION TYPE

This section in the settings is only available for some products. Search for “Inflow” on the page: http://www.comsol.com/products/specifications/ for more details on availability.

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints. The other option, **Flux (Danckwerts)** can be more stable and fast to solve when high reaction rates are anticipated in the vicinity of the inlet. Oscillations on the solutions can also be avoided in such cases. The latter condition uses a flux boundary condition based on the velocity across the boundary and the concentration values. See further details in the theory section.

#### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms 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 are the dominating transport mechanisms across the boundary, and therefore that the diffusive transport can be ignored, that is:

$$\mathbf{n} \cdot (-D\nabla c) = 0$$

Note that the **Convection** or the **Migration in electric field** transport mechanisms needs to be included for this node to be available.

## *Concentration*

This condition node adds a boundary condition for the species concentration. For example, a $c = c_0$ condition specifies the concentration of species $c$.

### CONCENTRATION

Individually specify the concentration for each species. Select the check box for the **Species** to specify the concentration, and then enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the check box for the concentration of that species.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

## *Flux*

This node can be used to specify the species flux across a boundary. The prescribed flux of a species $c$ is defined as:

$$-\mathbf{n} \cdot (-D\nabla c) = J_0$$

When the mass transport includes migration of ionic species, the flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi) = J_0$$

The flux prescribed, $J_0$, is an arbitrary user-specified flux expression. It can for example represent a flux due to chemical reactions or phase change, or the transport to or from a surrounding environment currently not included model. $J_0$ can be constant or a function of the any dependent variable, for example the concentration, temperature, pressure or the electric potential $\phi$.

#### INWARD FLUX

Select the Species check box for the species to specify 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:

$$-\mathbf{n} \cdot [(\mathbf{J} + \mathbf{u}c)_u - (\mathbf{J} + \mathbf{u}c)_d] = N_0 \qquad \mathbf{J} = -D\nabla c$$

where the value $N_0$ (SI unit: $\text{mol}/(\text{m}^2\cdot\text{s})$) 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 ratio between the concentration of a solute species in two different 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. For a species concentration $c_i$, the ratio between the concentration on the up side and on the down side of the boundary ($c_{i,\mathrm{u}}$ and $c_{i,\mathrm{d}}$ respectively) is defined as

$$K_i = \frac{c_{i,\,\mathrm{u}}}{c_{i,\,\mathrm{d}}}$$

in terms of a partition coefficient $K_i$. The up and down side of the selected boundary is indicated in the Graphics window. The arrows point from the down side into the up side.

! This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

### PARTITION COEFFICIENT

Select the **Reverse direction** check box to reverse the direction of the arrows on the selected boundaries, and the corresponding definition of the up and down side concentration.

Use the associated input fields to prescribe the partition coefficient $K_i$.

#### FURTHER READING

For an example of using a partition condition, see this application example:

*Separation Through Dialysis*: Application Library path **Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis**

## Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the mass transport between two sets of boundaries. The node prescribes continuity in the concentration and the mass flux between the "source" and the "destination" side respectively. Note that these names are arbitrary and does not influence the direction in which mass is transported. It is dictated by mass transfer equations in the adjacent domains.

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

For more complex geometries, it might be necessary to add the **Destination Selection** subnode, which is available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu. With this subnode, the boundaries that constitute the source and destination surfaces can be manually specified.

#### FURTHER READING

For an example of using a periodic condition, see this application example:

*The KdV Equation and Solitons*: Application Library path **COMSOL_Multiphysics/Equation_Based/kdv_equation**

## Line Mass Source

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

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

### SELECTION

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

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

### SPECIES SOURCE

Enter the source strength, $\dot{q}_{\mathrm{l,c}}$, for each species (SI unit: mol/(m·s)). A positive value results in species injection from the line into the computational domain, and a negative value means that the species is removed from the computational domain.

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

### FURTHER READING

See the section Mass Sources for Species Transport.

## Point Mass Source

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

!

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

### SPECIES SOURCE

Enter the source strength, $\dot{q}_{\mathrm{p,c}}$, for each species (SI unit: mol/s). A positive value results in species injection from the point into the computational domain, and a negative value means that the species is removed from the computational domain.

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

#### FURTHER READING

See the section Mass Sources for Species Transport.

## *Open Boundary*

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 http://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 an equilibrium reaction, involving two or more species, in a domain. Note that a necessary requirement for this is feature to be available is that two or more species are solved for by the interface.

The equilibrium reaction is defined by the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition) and the stoichiometry of the reaction.

The node solves for an additional degree of freedom (the reaction rate) to fulfill the equilibrium condition at all times in all space coordinates.

If the **Apply equilibrium condition on inflow boundaries** check box is selected, the specified inflow concentration values in all active **Inflow** boundary nodes for the physics interface are modified to comply with the equilibrium condition.

! This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

### EQUILIBRIUM CONDITION

The list defaults to **Equilibrium constant** or select **User defined**. For either option, the **Apply equilibrium condition on inflow boundaries** check box is selected by default.

For **Equilibrium constant**, enter an **Equilibrium constant** $K_{\mathrm{eq}}$ (dimensionless). The default is 1. Enter a value or expression for the **Unit activity concentration** $C_{\mathrm{a0}}$ (SI unit: mol/m$^3$). The default is $1{\cdot}10^{-3}$ mol/m$^3$. **Equilibrium constant** creates an equilibrium condition based on the stoichiometric coefficients, the species activities, and the law of mass action.

For **User defined**, enter an **Equilibrium expression** $E_{\mathrm{eq}}$ (dimensionless).

### STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient $\nu_{\mathrm{c}}$ (dimensionless). The default is 0. Use negative values for reactants and positive values for products in the modeled reaction.

Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium Reaction** node.

## Surface Reactions

The **Surface Reactions** node can be used to account for the species boundary flux due to chemical reactions occurring on a surface (heterogeneous reactions). For a domain species participating in a surface reaction, the boundary flux corresponds to the reaction rate at the surface.

### SURFACE REACTION RATE

Specify the surface reaction rate $J_0$ of each species resulting from the reactions. Note that if you have the Chemistry interface available, provided with the Chemical Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down menu.

### FURTHER READING

For an example of using the Surface Reactions node, see this application example:

*Chemical Vapor Deposition of GaAs*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/gaas_cvd**

## Surface Equilibrium Reaction

Use this node to model an equilibrium reaction on a boundary (surface). The settings for this node are similar to Equilibrium Reaction. Note that a necessary requirement for this is feature to be available is that two or more species are solved for by the interface.

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

### *Fast Irreversible Surface Reaction*

This boundary node defines an irreversible reaction where the kinetics is so fast that the only factor limiting the reaction rate is the transport of a species to the reacting surface.

The node will set the **Rate limiting species concentration to zero** at the boundary, and balance the fluxes of the species participating in the reaction and the current densities according to the Stoichiometric Coefficients settings.

| | |
|---|---|
| ! | This feature is only available in a limited set of add-on products. See http://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 Electrode Reaction nodes of an Electrochemistry Interface.

The molar source is calculated from the number of electrons, stoichiometric coefficients, and volumetric current densities of the coupled porous electrode reactions specified in the **Reaction Coefficients** subnodes.

In the Transport of Concentrated Species interface, the molar sources (or sinks) are multiplied by the species molar masses to obtain the corresponding mass sources.

Additional Reaction Coefficients subnodes are available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Note that if you are also modeling the momentum transport and expect a non-negligible total mass source or sink, which is often the case in gas diffusion electrodes, you need to also add a corresponding Porous Electrode Coupling node in the Fluid Flow interface.

| | |
|---|---|
| ! | This feature is only available in a limited set of add-on products. See http://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** ($i_{\mathrm{loc}}$, SI unit: $\mathrm{A/m^2}$) or **Porous Electrode Reaction** nodes ($i_{\mathrm{v}}$, SI unit: $\mathrm{A/m^3}$) of any **Electrochemistry** interface in the model are available for selection as the **Coupled reaction**, and user-defined expressions are also supported.

Enter the **Number of participating electrons** $n_m$ (dimensionless) and the **Stoichiometric coefficient** $v_c$ (dimensionless) as explained in the theory section linked below.

Use multiple subnodes to couple to multiple reactions.

## *Electrode Surface Coupling*

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 non-negligible total mass flux over the boundary, which is often the case for gas diffusion electrodes, you need to also add a corresponding Electrode Surface Coupling node in the Fluid Flow interface.

| | |
|---|---|
| ! | This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability. |

### *Porous Media Transport Properties*

Use this node to model the concentration of diluted species transported through interstices in porous media. A part form convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and reaction.

| | |
|---|---|
| ! | This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability. |

#### MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

#### MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Domain material** is used.

Specify the **Porosity,** $\varepsilon_\mathrm{p}$ (dimensionless) of the porous matrix. This is by default taken **From material**. Select **User defined** to instead enter a different value.

#### CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

#### DIFFUSION

Select a **Fluid material** (when available and applicable).

Specify the **Fluid diffusion coefficient** $D_{\mathrm{F,i}}$ (SI unit: m$^2$/s). Enter a value or expression for each of the species in the corresponding input field. The default is $1\cdot10^{-9}$ m$^2$/s.

Select the **Effective diffusivity model**: **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{\mathrm{F,i}}$ (dimensionless). The default is 1.

#### MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

- Enter a value or expression for the **Electric potential** $V$, which is **User defined**; this input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has also been added to the model.
- Select the electric potential defined or solved by Electrochemistry interface that has been added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, and under **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** — and type in the value of expression of the effective mobility $u_{\mathrm{me,c.}}$

Enter the **Charge number** $z_{\mathrm{c}}$ for each species.

#### DISPERSION

This section is available when the **Dispersion in porous media** check box is selected on the **Settings** window for the physics interface.

Select the **Specify dispersion for each species individually** check box to specify the dispersion tensor $D_{\mathrm{D}}$ (SI unit: m$^2$/s) for each species separately. The default is to use the same dispersion tensor $D_{\mathrm{D}}$ for all species.

Select an option from the **Dispersion tensor** list — **User defined** (the default) or **Dispersivity**. For **User defined**, use it to specify the dispersion components as user-defined constants or expressions. Select **Isotropic**, **Diagonal**, **Symmetric**, or **Anisotropic** based on the properties of the dispersion tensor.

Select **Dispersivity** when **Convection** has been added as the transport mechanism. Specify the dispersivities (SI unit: m) to define the dispersion tensor $D_{\mathrm{D}}$ (SI unit: m$^2$/s) together with the velocity field $\mathbf{u}$. Select an option from the **Dispersivity model** list: **Isotropic** (the default) or **Transverse isotropic** based on the properties of the porous media. For isotropic porous media, specify the longitudinal and transverse dispersivities. For transverse isotropic porous media, specify the longitudinal, horizontal transverse, and vertical transverse dispersivities.

## *Adsorption*

Use this node to model adsorption of the fluid phase species onto the porous media surface. It is available as a subnode to the Porous Media Transport Properties and the Partially Saturated Porous Media nodes.

> ! This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

### MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Domain material** is used.

The density of the porous media is needed when modeling adsorption to the surface of the porous matrix. By default **Density** $\rho$ is defined from the domain material.

### ADSORPTION

Select a **Sorption type** — **Langmuir** (the default), **Freundlich**, or **User defined** to specify how to compute $c_{\mathrm{P}}$, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

- For **Langmuir**:

$$c_{\mathrm{P}} = c_{\mathrm{Pmax}}\frac{K_{\mathrm{L}}c}{1+K_{\mathrm{L}}c} \qquad \frac{\partial c_{\mathrm{P}}}{\partial c} = \frac{K_{\mathrm{L}}c_{\mathrm{Pmax}}}{(1+K_{\mathrm{L}}c)^2}$$

  Enter a **Langmuir constant** $k_{\mathrm{L,c}}$ (SI unit: $\mathrm{m}^3/\mathrm{mol}$) and an **Adsorption maximum** $c_{\mathrm{p,max,c}}$ (SI unit: mol/kg):

- For **Freundlich**:

$$c_\mathrm{P} = K_\mathrm{F}\left(\frac{c}{c_\mathrm{ref}}\right)^N \qquad \frac{\partial c_\mathrm{P}}{\partial c} = N\frac{c_\mathrm{P}}{c} \qquad \text{Freundlich}$$

Enter a **Freundlich constant** $k_{\mathrm{F,c}}$ (SI unit: mol/kg), a **Freundlich exponent** $N_{\mathrm{F,c}}$ (dimensionless), and a **Reference concentration** $c_{\mathrm{ref,c}}$ (SI unit: mol/m$^3$).

- For **User defined**:

$$c_\mathrm{P} = K_P c \qquad \frac{\partial c_\mathrm{P}}{\partial c} = K_P \qquad \text{User defined}$$

Enter an **Adsorption isotherm** $k_{\mathrm{P,c}}$ (SI unit: m$^3$/kg).

For more information, see Adsorption in the theory section.

#### FURTHER READING

See the theory chapter in the section Mass Balance Equation for Transport of Diluted Species in Porous Media.

### *Partially Saturated Porous Media*

Use this node to model the concentration of diluted species transported by a liquid through in partially filled porous media. The interstices of the porous media contains the liquid carrier phase and gas pockets. A part from convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, reaction, and volatilization.

| | |
|---|---|
| ! | This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability. |

#### MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

### MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Domain material** is used.

Specify the **Porosity,** $\varepsilon_{\mathrm{p}}$ (dimensionless) of the porous matrix. This is by default taken **From material**. Select **User defined** to instead enter a different value.

### SATURATION

Select **Saturation** or **Liquid volume fraction** from the list.

For **Saturation**, enter a value for $s$ (dimensionless) between 0 and 1. The liquid volume fraction is then computed from the saturation and porosity as $\theta = s\varepsilon_{\mathrm{p}}$.

For **Liquid volume fraction**, enter a value for $\theta$ (dimensionless) between 0 and the value of porosity. The saturation is then computed from the porosity and the liquid volume fraction as $s = \theta\varepsilon_{\mathrm{p}}$.

Select a **Fluid fraction time change**: **Fluid fraction constant in time** (the default), **Time change in fluid fraction**, or **Time change in pressure head**.

- For **Time change in fluid fraction**, enter $\mathrm{d}\theta/\mathrm{d}t$ (SI unit: 1/s).
- For **Time change in pressure head**, enter $\mathrm{d}H_{\mathrm{p}}/\mathrm{d}t$ (SI unit: m/s) and a **Specific moisture capacity** $C_{\mathrm{m}}$ (SI unit: 1/m).

### CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

### DIFFUSION

Select a **Liquid material** from the list.

Specify the **Liquid diffusion coefficient** $D_{\mathrm{L,c}}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$). Enter a value or expression for each of the species in the corresponding input field. The default is $1{\cdot}10^{-9}\ \mathrm{m}^2/\mathrm{s}$.

Select the **Effective diffusivity model, liquid**: **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined**. For **Tortuosity model**, enter a value for $\tau_{\mathrm{L,c}}$ (dimensionless). The default is 1.

When the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface, also define the **Gas material**, **Gas diffusion coefficient**, and **Effective diffusivity model, gas**.

#### MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. It is similar to that in **Porous Media Transport Properties** feature. Select the source of electric field from the **Electric potential** list. The default selection to **Mobility** is the **Nernst-Einstein relation**.

#### DISPERSION

This section is available when the **Dispersion in porous media** check box is selected on the **Settings** window for the physics interface. The settings are the same as for Porous Media Transport Properties.

#### VOLATILIZATION

This section is available when the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface.

Enter a value for the **Volatilization** $k_{\mathrm{G,c}}$ (dimensionless) for each species.

### *Volatilization*

This feature is available when the **Volatilization in partially saturated porous media** check box is selected on the **Settings** window for the physics interface.

Use this feature to model mass transfer at the boundary due to volatilization. The feature can be added on boundaries of a **Partially Saturated Porous Media** domain. In this case the porous media contains a liquid phase and a gas phase. 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

$$-\mathbf{n}\cdot\mathbf{J}_{\mathrm{c}} = -h_{\mathrm{c}}(k_{\mathrm{G,c}}c - c_{\mathrm{Gatm,c}})$$

where $h_c$ is the mass transfer coefficient, $k_{G,c}$ the volatilization coefficient, and $c_{Gatm,c}$ the concentration in the surrounding atmosphere.

| | |
|---|---|
| ! | This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability. |

### VOLATILIZATION

Enter a **Mass transfer coefficient** $h_c$ defining the transfer into the surrounding media. This can be given by boundary layer theory. When assuming that no convective flow is present in the surrounding, the mass transfer coefficient can be defined from the gas diffusion coefficient $D_{Gc}$ and the thickness of the diffusion layer $d_s$ in the manner of

$$h_c = \frac{D_{Gc}}{d_s}$$

Also give the atmospheric concentration for each species, $c_{Gatm,c}$. The **Volatilization** coefficient $k_{G,c}$ for each species are taken from the adjacent **Partially Saturated Porous Media** domain.

## *Reactive Pellet Bed*

Use this feature to model packed bed reactors with catalytic pellets. For details, see the section Theory for the Reactive Pellet Bed. By default, subnodes for Reactions and  are added.

| | |
|---|---|
| ! | This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability. |

### BED PARAMETERS

Here you can specify the bed porosity, which is the void fraction in the packed bed structure. Select **From densities** to calculate the porosity from the bed density and the individual pellet density. Select **User defined** to specify the porosity directly.

### PELLET SHAPE AND SIZE

The default shape is spherical. Cylinders, flakes, and user-defined shapes can also be selected. A uniform pellet size or a discrete size distribution can be selected. Select a

**Pellet size distribution** — **Uniform size** (the default), **Two sizes**, **Three sizes**, **Four sizes**, or **Five sizes** to select up to five different particle sizes.

Depending on the shape selection, equivalent radii or volumes and surface areas will be required as input. If a size distribution is selected, the volume percentage of each size is required as input.

Note that different chemical reactions can be specified for each pellet size if a distribution is specified.

### SURFACE SPECIES

In order to add surface species, click the **Add** button and enter the species name in the **Surface species** table. Added surface species are be available inside all pellet types defined in the **Pellet Shape and Size** section, but not in the bulk fluid.

For each pellet type, specify the **Reactive specific surface area**, $S_{\mathrm{b,reac}}$ (SI unit: 1/m), corresponding to the surface area, per volume, available for surface reactions.

### PELLET PARAMETERS

Enter a **Pellet porosity** $\varepsilon_{\mathrm{pe}}$ (dimensionless) to specify the porosity of the pellet internals.

Select **Diffusion model** — **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **User defined** to describe the effective correction of the diffusion coefficient in the pellet. In the case of the **Tortuosity model**, a value for the tortuosity $\tau_{\mathrm{pe}}$ within the pellet is required.

Enter also the **Diffusion coefficient** $D_{\mathrm{pe,c}}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$). If a **User defined** diffusion model is selected, an **Effective diffusion coefficient** $D_{\mathrm{peff,c}}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$) is entered. The default value is $1{\cdot}10^{-9}$ $\mathrm{m}^2/\mathrm{s}$ in both cases.

### PELLET-FLUID SURFACE

For the coupling of concentration between the pellet internals and the surrounding fluid, two **Coupling type** options are available:

- **Continuous concentration***,* assuming that all resistance to mass transfer to/from the pellet is within the pellet and no resistance to pellet-fluid mass transfer is on the bulk fluid side. The concentration in the fluid will thus be equal to that in the pellet pore just at the pellet surface: $c_{\mathrm{pe},i} = c_i$ . This constraint also automatically ensures flux continuity between the internal pellet domain and the free fluid domain through so-called reaction forces in the finite element formulation.

- **Film resistance (mass flux)**: The flux of mass across the pellet-fluid interface into the pellet is possibly rate determined on the bulk fluid side, by film resistance. The resistance is expressed in terms of a film mass transfer coefficient, $h_{Di}$, such that:

$$N_{i,\text{inward}} = h_{D,i}(c_i - c_{\text{pe},i}) .$$

The **Film resistance (mass flux)** option computes the inward surface flux, $N_{\text{i,inward}}=h_{\text{Di}}(c_{\text{i}}\text{-}c_{\text{pe,i}})$. $h_{\text{Di}}$ is the mass transfer coefficient (SI unit: m/s) and is calculated with the default **Automatic** setting from a dimensionless **Sherwood number expression** or with **User defined** mass transfer coefficients.

The **Active specific surface area** (SI unit: $\text{m}^{-1}$) is required to couple the mass transfer between the pellets and the bed fluid. Select either the **Automatic** setting that calculates the specific surface area from the shape information given above. User defined is also available for explicit surface area specification.

The **Sherwood number expression** can be computed from three available expressions: **Frössling**, **Rosner**, and **Garner and Keey**. The Frössling equation is the default and probably the most commonly used for packed spheres. All of these are based on the dimensionless Reynolds, Re, and Schmidt, Sc, numbers, which are computed from **Density** and **Dynamic viscosity**. Select these to be taken either **From material** or choose the **User defined** alternative.

### PELLET DISCRETIZATION

The extra dimension in the pellet needs to be discretized into elements. Select a **Distribution** — **Cubic root sequence** (the default), **Linear**, or **Square root sequence**. Enter the **Number of elements** $N_{\text{elem}}$.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( 👁 ) and select **Advanced Physics Options**. See the details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

### FURTHER READING

Theory for the Reactive Pellet Bed in the Theory section of this manual.

For an application using the Reactive Pellet Bed feature, see

- *A Multiscale 3D Packed Bed Reactor*: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/packed_bed_reactor_3d**

  Web link: http://www.comsol.com/model/a-multiscale-3d-packed-bed-reactor-17019

## Reactions

The Reactions subfeature to the Reactive Pellet Bed is used to define reaction terms to the transport within the reactive pellets. The feature also defines the corresponding averaged heat sources to be applied to heat transport in the bulk fluid.

### DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern source terms in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

### REACTION RATES

Add a rate expression $R$ (SI unit: mol/(m$^3$·s)) for species $i$ using a value or an expression. One reaction rate per species and pellet type can be entered.

Note that if you have the *Chemistry* interface available, provided with the *Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down menu. For an example, see the application *Fine Chemical Production in a Plate Reactor*.

### SURFACE REACTION RATES

The section is available when one or more surface species have been added in the **Surface Species** section of the Reactive Pellet Bed feature.

Specify the rate expression $R$ (SI unit: mol/(m$^2$·s)) corresponding to the surface reaction rate of each volumetric species $i$ participating in the surface reaction. Furthermore, specify the surface reaction rates for the participating surface species in the corresponding table.

If several pellet types have been defined, one set of surface reaction rates per pellet type can be defined.

Note that if you have the *Chemistry* interface available, provided with the *Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down menu.

#### HEAT SOURCE

Specify the heat source originating from the heat of reaction of the chemical reactions inside the pellet can be specified. Both heat sources from reactions in the fluid, and heat sources resulting from surface reactions can be defined. When using several pellet types, heat sources for each type can be added.

The heat sources are most conveniently picked up from a Chemistry feature that defines the reaction rate and the heat of reactions. In that case, the Rate expression can be selected from the drop-down menu. Else it can be set to User Defined.

The defined heat source can be used by a Heat Source feature in any of the heat transfer interfaces.

### *Species Source*

In order to account for consumption or production of species in porous domains, the **Species Source** node adds source terms expressions $S_i$ to the right-hand side of the species transport equations.

#### DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

If there are several types of domains, with subsequent and different reactions occurring within them, it might be necessary to remove some domains from the selection. These are then defined in an additional **Species Source** node.

#### SPECIES SOURCE

Add a source term $S_i$ (SI unit: $\mathrm{mol/(m^3{\cdot}s)}$) for each of the species solved for. Enter a value or expression in the field of the corresponding species.

## Hygroscopic Swelling

The **Hygroscopic Swelling** multiphysics coupling node ( ) is used for moisture concentration coupling between the Solid Mechanics interface and either the Transport of Diluted Species or Transport of Diluted Species in Porous Media interfaces.

Hygroscopic swelling is an effect of internal strain caused by changes in moisture content. This strain can be written as

$$\varepsilon_{\mathrm{hs}} = \beta_h M_m (c_{\mathrm{mo}} - c_{\mathrm{mo,ref}})$$

where $\beta_{\mathrm{h}}$ is the coefficient of hygroscopic swelling, $M_{\mathrm{m}}$ is the molar mass, $c_{\mathrm{mo}}$ is the moisture concentration, and $c_{\mathrm{mo,ref}}$ is the strain-free reference concentration.

It requires a license of either the MEMS Module or the Structural Mechanics Module. The multiphysics feature will appear automatically if both the Transport of Diluted Species and the Solid Mechanics interfaces are added to the same component. For the most current information about licensing, please see See http://www.comsol.com/products/specifications/.

### FURTHER READING

More information about how to use hygroscopic swelling can be found in Hygroscopic Swelling Coupling section in the *Structural Mechanics Module User's Guide*.

More information about multiphysics coupling nodes can be found in the section The Multiphysics Branch in the *COMSOL Multiphysics Reference Manual*.

## Fracture

Use this node to model mass transport along thin fractures in porous media. The node assumes that the transport in the tangential direction along the fracture is dominant, as a result of lower flow resistance.

!

This feature is only available in a limited set of add-on products. See http://www.comsol.com/products/specifications/ for more details on availability.

### FRACTURE PROPERTIES

Specify a value for the **Fracture thickness** $d_{\mathrm{fr}}$.

#### MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Boundary material** is used.

Specify the **Porosity,** $\varepsilon_\mathrm{p}$ (dimensionless) of the porous matrix. This is by default taken **From material**. Select **User defined** to instead enter a different value.

#### CONVECTION

Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use a Fracture Flow feature in a Darcy's Law interface to compute the fluid flow velocity in the fracture.

For **User defined**, enter values or expressions for the velocity components in the table shown.

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The settings for the **Diffusion**, and **Dispersion** sections are the same as for Porous Media Transport Properties.

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# The Transport of Diluted Species in Fractures Interface

The **Transport of Diluted Species in Fractures (dsf)** interface ( ), 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 http://www.comsol.com/products/specifications/

#### SETTINGS

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

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

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

#### BOUNDARY SELECTION

If model geometry includes boundaries that should not be included in the mass transfer simulation, remove those from the selection list.

#### TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the **Convection** check box, available under **Additional transport mechanisms**, to control whether to also include convective transport.

### CONSISTENT STABILIZATION

To display this sections, click the **Show** button ( ) 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** $g_{\mathrm{lim}}$. It defaults to `0.1[mol/m^3)/tds.helem`, where `tds.helem` is the local element size.
- For both consistent stabilization methods select an **Equation residual**. **Approximate residual** is the default and means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is computationally faster. If required, select **Full residual** instead.

### INCONSISTENT STABILIZATION

To display this section, click the **Show** button ( ) and select **Stabilization**. By default, the **Isotropic diffusion** check box is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for underresolved problems.

### DISCRETIZATION

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

The **Value type when using splitting of complex variables** setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

### DEPENDENT VARIABLES

The dependent variable name is **Concentration** c by default. A dependent variable name must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the **Number of species**. Use the **Add concentration** ( + ) and **Remove concentration** ( ) buttons as needed.

### FURTHER READING

- Mass Transport in Fractures in the theory section.
- Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*.
- Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface
- In the *COMSOL Multiphysics Reference Manual*, see Table 2-3 for links to common sections and Table 2-4 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

## *Boundary, Edge, Point, and Pair Nodes for the Transport of Diluted Species in Fractures Interface*

The Transport of Diluted Species in Fractures Interface has the following boundary, edge, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- Adsorption
- Concentration
- Flux
- Fracture
- Inflow
- Initial Values
- No Flux
- Outflow
- Reactions
- Species Source

## *Adsorption*

Use this node to model adsorption of the fluid phase species in onto the porous media surface of the fracture.

### MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Domain material** is used. The density of the porous media is needed when modeling adsorption to the surface of the porous matrix. By default **Density** $\rho$ is set to from domain material.

adsorption

Select a **Sorption type**—**Langmuir** (the default), **Freundlich**, or **User defined** to specify how to compute $c_\mathrm{P}$, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

- For **Langmuir**:

$$c_\mathrm{P} = c_\mathrm{Pmax}\frac{K_\mathrm{L}c}{1+K_\mathrm{L}c} \qquad \frac{\partial c_\mathrm{P}}{\partial c} = \frac{K_\mathrm{L}c_\mathrm{Pmax}}{(1+K_\mathrm{L}c)^2}$$

  Enter a **Langmuir constant** $k_{\mathrm{L,c}}$ (SI unit: m$^3$/mol) and an **Adsorption maximum** $c_{\mathrm{p,max,c}}$ (SI unit: mol/kg):

- For **Freundlich**:

$$c_\mathrm{P} = K_\mathrm{F}\left(\frac{c}{c_\mathrm{ref}}\right)^N \qquad \frac{\partial c_\mathrm{P}}{\partial c} = N\frac{c_\mathrm{P}}{c} \qquad \text{Freundlich}$$

  Enter a **Freundlich constant** $k_{\mathrm{F,c}}$ (SI unit: mol/kg), a **Freundlich exponent** $N_{\mathrm{F,c}}$ (dimensionless), and a **Reference concentration** $c_{\mathrm{ref,c}}$ (SI unit: mol/m$^3$).

- For **User defined**:

$$c_\mathrm{P} = K_P c \qquad \frac{\partial c_\mathrm{P}}{\partial c} = \frac{\partial}{\partial c}(K_P c) \qquad \text{User defined}$$

  Enter an **Adsorption isotherm** $k_{\mathrm{P,c}}$ (SI unit: m$^3$/kg).

For more information, see Adsorption in the theory section.

### FURTHER READING

See the theory chapter in the section Mass Balance Equation for Transport of Diluted Species in Porous Media.

## *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 ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

## *Flux*

This node can be used to specify the species flux across a boundary of a porous fracture (applied in points in 2D and along edges in 3D). The flux of species $c$ is defined as

$$\mathbf{n} \cdot (D_e \nabla c) = N_0$$

where $N_0$ is an arbitrary user-specified flux expression. For example, $N_0$ can represent a flux due to chemical reactions, or a phase change. A positive $N_0$ implies that the concentration inside the fracture increases.

### INWARD FLUX

Specify the flux of each species individually. To use another boundary condition for a specific species, click to clear the check box for the mass fraction of that species.

## *Fracture*

Use this node to model mass transport along thin fracture surfaces situated inside porous or solid material. The node assumes that the transport in the tangential direction of the fracture is dominant, as a result of lower flow resistance. Note that the fracture it self is modeled as porous.

### MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Boundary material** is used.

Specify the **Porosity,** $\varepsilon_p$ (dimensionless) of the porous matrix. This is by default taken **From material**. Select **User defined** to instead enter a different value.

### CONVECTION

Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use The Fracture Flow Interface to compute the fluid flow velocity.

For **User defined**, enter values or expressions for the velocity components in the table shown.

The settings for the **Diffusion**, and **Dispersion** sections are the same as for Porous Media Transport Properties.

## *Inflow*

Use this node to specify all species concentrations at a fracture inlet. The condition is applied in points in 2D and along edges in 3D

If you want to specify the concentration of a subset of the partaking species, this can be done by using the Concentration node instead.

### CONCENTRATION

For the concentration of each species $c_{0,c}$ (SI unit: mol/m$^3$), enter a value or expression.

### BOUNDARY CONDITION TYPE

This section in the settings is only available for some products. Search for “Inflow” on the page: http://www.comsol.com/products/specifications/ for more details on availability.

The option **Concentration constraint** constrains the concentration values on the boundary by the use of pointwise constraints. The other option, **Flux (Danckwerts)** can be more stable and fast to solve when high reaction rates are anticipated in the vicinity of the inlet. Oscillations on the solutions can also be avoided in such cases. The latter condition uses a flux boundary condition based on the velocity across the boundary and the concentration values. See further details in the theory section.

### CONSTRAINT SETTINGS

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms 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:

$$\mathbf{n} \cdot (-D_{\mathrm{e}} \nabla c) = 0$$

## 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, provided with the *Chemical Reaction*

*Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down menu.

### REACTING VOLUME

When specifying reaction rates for a species in a fracture, the specified reaction rate may have the basis of the pore volume of the fracture, or the total volume.

- For **Total volume**, the reaction expressions in are specified per unit volume of the fracture. The reaction expressions will be multiplied by the fracture thickness $d_{\mathrm{fr}}$.
- For **Pore volume**, the reaction expressions in mol/(m$^3$·s) are specified per unit volume of total pore space in the fracture. The reaction expressions will be multiplied by the fracture thickness $d_{\mathrm{fr}}$ and the fracture porosity, $\varepsilon_{\mathrm{p}}$.

## *Species Source*

In order to account for consumption or production of species in a fracture, the **Species Source** node adds source terms expressions $S_i$ to the right-hand side of the species transport equations.

### BOUNDARY SELECTION

From the **Selection** list, choose the boundaries on which to define expressions that govern the source term in the transport equations.

If there are several different parts of the fracture, with subsequent and different sources occurring within them, it might be necessary to remove some boundaries from the selection. The sources in these can then be defined using an additional **Species Source** node.

### SPECIES SOURCE

Add a source term $S_i$ for each of the species solved for. Enter a value or expression in the field of the corresponding species.

# Theory for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution of chemical species transported by diffusion and convection. The physics interface assumes that all species present are dilute; that is, that their concentration is small compared to a solvent fluid or solid. As a rule of thumb, a mixture containing several species can be considered dilute when the concentration of the solvent is more than 90 mol%. Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent.

When studying mixtures that are not dilute, the mixture and transport properties depend on the composition, and a different physics interface is recommended. See The Transport of Concentrated Species Interface 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:

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 $i$:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i \tag{4-1}$$

Equation 4-1 in its form above includes the transport mechanisms diffusion and convection. If *Migration in Electric Field* is activated (only available in some add-on products), the migration mechanism will be added to the equation as well. See more details in the section Adding Transport Through Migration.

- $c_i$ is the concentration of the species (SI unit: mol/m$^3$)
- $D_i$ denotes the diffusion coefficient (SI unit: m$^2$/s)
- $R_i$ is a reaction rate expression for the species (SI unit: mol/(m$^3$·s))
- $\mathbf{u}$ is the mass averaged velocity vector (SI unit: m/s)

The mass flux diffusive flux vector

The mass flux relative to the mass averaged velocity, $\mathbf{J}_i$ (SI unit: mol/(m$^2$·s)), is associated with the mass balance equation above and used in boundary conditions and flux computations. The Transport of Diluted Species interface always includes mass transport due to molecular diffusion. In this case the mass flux $\mathbf{J}_i$ defines the diffusive flux vector

$$\mathbf{J}_i = -D\nabla c \tag{4-2}$$

An input field for the diffusion coefficient is available. Anisotropic diffusion tensor input is supported.

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 4-1 describes the convective transport due to a velocity field $\mathbf{u}$. 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 4-1), $R_i$ represents a source or sink term, typically due to a chemical reaction or desorption on a porous matrix. To specify $R_i$, another node must be added to the Transport of Diluted Species interface — the **Reaction** node 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, $\nu_i$ (dimensionless), of the reaction; the species activities of the reacting species $a_i$ (dimensionless); and an equilibrium constant, $K_{\mathrm{eq}}$ (1) according to:

$$K_{\mathrm{eq}} = \frac{\displaystyle\prod_{i \in \text{products}} a_i^{\nu_i}}{\displaystyle\prod_{i \in \text{reactants}} a_i^{-\nu_i}}$$

where the species activities are defined as

$$a_i = \gamma_{c,i}\frac{c_i}{c_{\mathrm{a0}}}$$

where $c_{\mathrm{a0}}$ (SI unit: mol/m$^3$) is the standard molarity, and $\gamma_{c,i}$ (dimensionless) an activity coefficient.

Defining the stoichiometric coefficients positive for products and negative for reactants, the above equilibrium condition can also be written:

$$K_{\mathrm{eq}} = \prod_i a_i^{\nu_i}$$

$\gamma_{c,i}$ is set to unity when the Equilibrium constant is selected on the Settings window. For nonunity activity coefficients, a user defined equilibrium condition can be used.

#### EQUILIBRIUM REACTIONS AND INFLOW BOUNDARY CONDITIONS

Contradictory constraints arise if the boundary conditions for concentrations or activities are set so that the domain equilibrium condition is not fulfilled. Special treatment is therefore needed at Inflow boundaries, where the concentrations are set for all species in the mass transport interfaces.

One way of avoiding competing constraints on an inflow boundary is to add an additional reaction coordinate degree of freedom, solved for to create a set of modified inflow concentrations that fulfill the domain equilibrium condition. The reaction coordinate gives rise to a concentration shift, which is the offset to the inflow concentrations provided by the user. The shift for each species obeys the stoichiometry of the reaction and the equilibrium expression. The modified inflow concentrations are then used in the boundary conditions for the domain mass transport equations. The resulting modified inflow concentrations can be seen as the stationary solution for a batch reactor with the user inflow concentrations as initial concentrations. In addition, the domain reaction rate degree of freedom of the equilibrium reaction is constrained to zero on all Inflow boundaries.

#### EQUILIBRIUM REACTIONS AND CONCENTRATION BOUNDARY CONDITIONS

No special treatment is made with regards to input concentration values of the Concentration boundary node. Using this feature, you can explicitly set one or a set of concentrations, and the equilibrium condition acts on the rest of the concentrations. However, there is no solution to the problem if more concentrations than the number of species minus the number of equilibrium reactions are set using this feature.

#### EQUILIBRIUM REACTIONS AND TIME-DEPENDENT SIMULATIONS

Spurious oscillations may occur in a time-dependent problem if the initial conditions do not fulfill the equilibrium condition. Since equilibrium reactions are assumed to be infinitely fast, the solution is to initialize the problem using an additional study step, solving for a stationary problem with all 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 and implements the mass balance equation in Equation 4-1.

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:

$$\text{nonconservative: } \frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = \nabla\cdot\mathbf{J}_i + R \tag{4-3}$$

$$\text{conservative: } \frac{\partial c}{\partial t} + \nabla\cdot(c\mathbf{u}) = \nabla\cdot\mathbf{J}_i + R \tag{4-4}$$

and each is treated slightly differently by the solver algorithms. In these equations $\mathbf{J}_i$ (SI unit: mol/(m$^2$·s)) is the diffusive flux vector, $R$ (SI unit: mol/(m$^3$·s)) is a production or consumption rate expression, and $\mathbf{u}$ (SI unit: m/s) is the solvent velocity field. The diffusion process can be anisotropic, in which case $D$ is a tensor.

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c\nabla\cdot\mathbf{u}$, would equal zero for an incompressible fluid and would result in the nonconservative formulation above. This is in fact the default formulation in this physics interface. To switch between the two formulations, click the **Show** button ( 👁 ) and select **Advanced Physics Options**.

## *Solving a Diffusion Equation Only*

Remove the convection term from Equation 4-3 and Equation 4-4 by clearing the Convection check box in the Transport Mechanisms section for The Transport of Diluted Species Interface. The equation then becomes

$$\frac{\partial c}{\partial t} = \nabla\cdot\mathbf{J}_i + R$$

## *Mass Sources for Species Transport*

There are two types of mass sources in the Transport of Diluted Species interface: point sources and line sources.

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**Note:** The features below are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit http://www.comsol.com/products/specifications/

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### POINT SOURCE

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

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q}_{\mathrm{c}} = \dot{q}_{\mathrm{p,c}} \tag{4-5}$$

An alternative way to form a point source is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant results in the same point source. For this alternative approach, effects resulting from the physical object's volume need to be neglected.

The weak contribution

$$\dot{q}_{\mathrm{p,c}}\mathrm{test}(c)$$

is added at a point in the geometry. As can be seen from Equation 4-5, $\dot{Q}_{\mathrm{c}}$ must tend to plus or minus infinity as $\delta V$ tends to zero. This means that in theory the concentration also tends to plus or minus infinity.

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

The finite element representation of Equation 4-5 corresponds to a finite concentration at a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region but also a more extreme concentration value. It is important not to mesh too finely around a point source since this can result in unphysical concentration values. It can also have a negative effect on the condition number for the equation system.

### LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}_{1,\mathrm{c}}$ (SI unit: mol/(m$^3$·s)), located within a tube with cross section $\delta S$ and then letting $\delta S$ tend to zero while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_{1,\mathrm{c}}$ (SI unit: mol/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q}_{1,\mathrm{c}} = \dot{q}_{1,\mathrm{c}} \qquad (4\text{-}6)$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects resulting from the physical object's volume are neglected.

The weak contribution

$$\dot{q}_{1,\mathrm{c}}\mathrm{test}(c)$$

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

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

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

## *Adding Transport Through Migration*

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**Note:** Migration is only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit http://www.comsol.com/products/specifications/

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In addition to transport due to convection and diffusion, the Transport of Diluted Species interface supports ionic species transport by *migration*. This is done by selecting the Migration in Electric Field check box under the Transport Mechanisms section for the physics interface. The mass balance then becomes:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V + c_i \mathbf{u}) = R_i \tag{4-7}$$

where

- $c_i$ (SI unit: mol/ m$^3$) denotes the concentration of species $i$
- $D_i$ (SI unit: m$^2$/s) is the diffusion coefficient of species $i$
- $\mathbf{u}$ (SI unit: m/s) is the fluid velocity
- $F$ (SI unit: A·s/mol) refers to Faraday's constant
- $V$ (SI unit: V) denotes the electric potential
- $z_i$ (dimensionless) is the charge number of the ionic species, and
- $u_{\mathrm{m},i}$ (SI unit: mol·s/kg) is its ionic mobility

In this case the diffusive flux vector is

$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V$$

The velocity, $\mathbf{u}$, can be a computed fluid velocity field from a Fluid Flow interface or a specified function of the spatial variables $x$, $y$, and $z$. The potential can be provided by an expression or by coupling the system of equations to a current balance, such as the Electrostatics interface. Sometimes it is assumed to be a supporting electrolyte present, which simplifies the transport equations. In that case, the modeled charged species concentration is very low compared to other ions dissolved in the solution. Thus, the species concentration does not influence the solution's conductivity and the net charge within the fluid.

The Nernst-Einstein relation can in many cases be used for relating the species mobility to the species diffusivity according to

$$u_{m,i} = \frac{D_i}{RT}$$

where $R$ (SI unit: J/(mol·K)) is the molar gas constant and $T$ (SI unit: K) is the temperature.

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**Note:** In the *Nernst-Planck Equations* interface, the ionic species contribute to the charge transfer in the solution. It includes an *electroneutrality condition* and also computes the electric potential field in the electrolyte. For more information, see Theory for the Nernst-Planck Equations Interface. This interface is included in the Chemical Reaction Engineering Module.

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### *Supporting Electrolytes*

In *electrolyte* solutions, a salt can be added to provide a high electrolyte conductivity and decrease the ohmic losses in a cell. These solutions are often called *supporting electrolytes*, buffer solutions, or carrier electrolytes. The added species, a negative and a positive ion pair, predominates over all other species. Therefore, the supporting electrolyte species can be assumed to dominate the current transport in the solution. In addition, the predominant supporting ions are usually selected so that they do not react at the electrode surfaces since the high conductivity should be kept through the process, that is, they should not be electro-active species. This also means that the concentration gradients of the predominant species in a supporting electrolyte are usually negligible.

Modeling and solving for a supporting electrolyte in the *Electrostatics* or *Secondary Current Distribution* interfaces will give a potential distribution that drives the migration in the Transport of Diluted Species Interface.

The current density vector is proportional to the sum of all species fluxes as expressed by Faraday’s law:

$$\mathbf{i} = F\sum_i z_i\mathbf{N}_i$$

The electroneutrality condition ensures that there is always a zero net charge at any position in a dilute solution. Intuitively, this means that it is impossible to create a current by manually pumping positive ions in one direction and negative ions in the other. Therefore, the convective term is canceled out to yield the following expression for the electrolyte current density, where $j$ denotes the supporting species:

$$\mathbf{i} = F\sum_j -z_j^2 u_{\mathrm{m},j} F c_j \nabla\phi \tag{4-8}$$

Equation 4-8 is simply Ohm's law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa\nabla\phi \tag{4-9}$$

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 4-9, yields:

$$\nabla\cdot(-\kappa\nabla\phi) = 0 \tag{4-10}$$

Equation 4-10 can be easily solved using the Electrostatics or Secondary Current Distribution interface and, when coupled to the Transport in Diluted Species interface, the potential distribution shows up in the migration term.

## *Crosswind Diffusion*

Transport of diluted species applications can often result in models with a very high cell Péclèt number—that is, systems where convection or migration dominates over diffusion. Streamline diffusion and crosswind diffusion are of paramount importance to obtain physically reasonable results. The Transport of Diluted Species interface provides two crosswind diffusion options using different formulations. Observe that crosswind diffusion makes the equation system nonlinear even if the transport equation is linear.

### DO CARMO AND GALEÃO

This is the formulation described in Numerical Stabilization. The method reduces over- and undershoots to a minimum, even for anisotropic meshes.

In some cases, the resulting nonlinear equation system can be difficult to converge. This can happen when the cell Péclèt number is very high and the model contains many thin layers, such as contact discontinuities. You then have three options:

- Refine the mesh, especially in regions with thin layers.
- Use a nonlinear solver with a constant damping factor less than one.
- Switch to the Codina crosswind formulation.

### CODINA

The Codina formulation is described in Ref. 1. It adds diffusion strictly in the direction orthogonal to the streamline direction. Compared to the do Carmo and Galeão formulation, the Codina formulation adds less diffusion but is not as efficient at reducing over- and undershoots. It also does not work as well for anisotropic meshes. The advantage is that the resulting nonlinear system is easier to converge and that underresolved gradients are less smeared out.

## *Danckwerts Inflow Boundary Condition*

Constraining the composition to fixed values at an inlet to a reactor may sometimes result in issues with unreasonably high reaction rates or singularities at the inlet boundary. These problems may many times be mitigated by using a flux boundary condition instead, based on the inlet concentrations and the fluid velocity. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet concentrations to domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an inlet concentration $c_{i,0}$, the Danckwerts inflow boundary condition reads

$$\mathbf{n}\cdot(\mathbf{J}_i+\mathbf{u}c_i) = \mathbf{n}\cdot(\mathbf{u}c_{i,\,0}) \qquad (4\text{-}11)$$

See further:

Inflow

## *Mass Balance Equation for Transport of Diluted Species in Porous Media*

### VARIABLY SATURATED POROUS MEDIA

The following equations for the molar concentrations, $c_i$, describe the transport of solutes in a variably saturated porous medium for the most general case, when the pore space is primarily filled with liquid but also contain pockets or immobile gas:

$$\frac{\partial}{\partial t}(\theta c_i)+\frac{\partial}{\partial t}(\rho c_{\mathrm{P},\,i})+\frac{\partial}{\partial t}(a_{\mathrm{v}} c_{\mathrm{G},\,i})+\mathbf{u}\cdot\nabla c_i = \nabla\cdot[(D_{\mathrm{D},\,i}+D_{\mathrm{e},\,i})\nabla c_i]+R_i+S_i \tag{4-12}$$

On the left-hand side of Equation 4-12, the first three terms correspond to the accumulation of species within the liquid, solid, and gas phases, while the last term describes the convection due to the velocity field $\mathbf{u}$ (SI unit: m/s).

In Equation 4-12 $c_i$ denotes the concentration of species $i$ in the liquid (SI unit: $\mathrm{mol/m^3}$), $c_{\mathrm{P},\,i}$ the amount adsorbed to solid particles (moles per unit dry weight of the solid), and $c_{\mathrm{G},\,i}$ the concentration of species $i$ in the gas phase.

The equation balances the mass transport throughout the porous medium using the porosity $\varepsilon_{\mathrm{p}}$, the liquid volume fraction $\theta$; the matrix (drained) density, $\rho = (1-\varepsilon_{\mathrm{p}})\rho_{\mathrm{p}}$, and the solid phase density $\rho_{\mathrm{p}}$.

For saturated porous media, the liquid volume fraction $\theta$ is equal to the porosity $\varepsilon_{\mathrm{p}}$, but for partially saturated porous media, they are related by the saturation $s$ as $\theta = s\varepsilon_{\mathrm{p}}$. The resulting gas volume fraction is $a_{\mathrm{v}} = \varepsilon_{\mathrm{p}} - \theta = (1\text{-}s)\varepsilon_{\mathrm{p}}$.

On the right-hand side of Equation 4-12, 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 $D_{\mathrm{D}}$ (SI unit: $\mathrm{m^2/s}$) and the effective diffusion by $D_{\mathrm{e}}$ (SI unit: $\mathrm{m^2/s}$).

The last two terms on the right-hand side of Equation 4-12 describe production or consumption of the species; $R_i$ is a reaction rate expression which can account for reactions in the liquid, solid, or gas phase, and $\mathrm{S}_i$ is an arbitrary source term, for example due to a fluid flow source or sink.

#### *Adsorption*

The time evolution of the adsorption, the solute transport to or from the solid phase, is defined by assuming that the amount of solute adsorbed to the solid, $c_{\mathrm{P},i,}$ is a function of the concentration in the fluid $c_{i.}$ This implies that the solute concentration in the liquid and solid phase are in instant equilibrium. The adsorption term can be expanded to give

$$\frac{\partial}{\partial t}(\rho c_{\mathrm{P},i}) = \rho\frac{\partial c_{\mathrm{P},i}}{\partial c_i}\frac{\partial c_i}{\partial t} - \rho c_{\mathrm{P},i}\frac{\partial \varepsilon_\mathrm{P}}{\partial t} = \rho k_{\mathrm{P},\mathrm{i}}\frac{\partial c_i}{\partial t} - \rho c_{\mathrm{P},i}\frac{\partial \varepsilon_\mathrm{P}}{\partial t} \tag{4-13}$$

where $k_{\mathrm{P},i} = \partial c_{\mathrm{P},i}/\partial c_i$ is the adsorption isotherm.

#### Volatilization

Volatilization is the process where a solute species in the liquid is transported to the gas phase due to vaporization. Assuming that the amount of solute in the gas phase, $c_{\mathrm{G},i}$, is a linear function of the liquid phase concentration, the volatilization term is defined as

$$\frac{\partial}{\partial t}a_\mathrm{v}c_{\mathrm{G},i} = a_\mathrm{v}\frac{\partial c_{\mathrm{G},i}}{\partial c_i}\frac{\partial c_i}{\partial t} + k_{\mathrm{G},i}c_i\frac{\partial a_\mathrm{v}}{\partial t} = a_\mathrm{v}k_{\mathrm{G},i}\frac{\partial c_i}{\partial t} + k_{\mathrm{G},i}c_i\frac{\partial a_\mathrm{v}}{\partial t} \tag{4-14}$$

where $k_{\mathrm{G},i} = \partial c_{\mathrm{G},i}/\partial c_i$ is the linear volatilization.

### SATURATED POROUS MEDIA

In the case of transport in a saturated porous medium, $\theta = \varepsilon_\mathrm{p}$, and the governing equations are

$$\frac{\partial}{\partial t}(\varepsilon_\mathrm{p}c_i) + \frac{\partial}{\partial t}(\rho c_{\mathrm{P},i}) + \mathbf{u}\cdot\nabla c_i = \nabla\cdot[(D_{\mathrm{D},i} + D_{\mathrm{e},i})\nabla c_i] + R_i + S_i \tag{4-15}$$

## 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 $\mathbf{u}$ 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:

$$\mathbf{u}_a = \frac{\mathbf{u}}{\varepsilon_p} \qquad \text{Saturated}$$

$$\mathbf{u}_a = \frac{\mathbf{u}}{\theta} \qquad \text{Partially saturated}$$

where $\varepsilon_p$ is the porosity and $\theta = s\varepsilon_p$ the liquid volume fraction, and $s$ the saturation, a dimensionless number between 0 and 1.

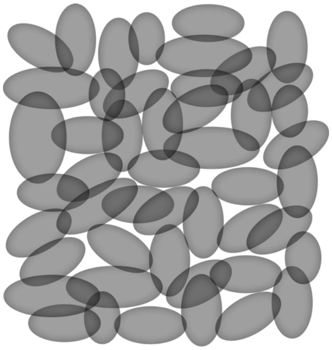

*Figure 4-1: A block of a porous medium consisting of solids and the pore space between the solid grains. The average linear velocity describes how fast the fluid moves within the pores. The Darcy velocity attributes this flow over the entire fluid-solid face.*

### CONVECTIVE TERM FORMULATION

The Transport of Diluted Species in Porous Media interface includes two formulations of the convective term. The conservative formulation of the species equations in Equation 4-12 is written as:

$$\begin{aligned}\frac{\partial}{\partial t}(\theta c_i) + \frac{\partial}{\partial t}(\rho_b c_{P,i}) + \frac{\partial}{\partial t}(a_v c_{G,i}) + \nabla \cdot \mathbf{u} c_i &= \\ \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_i] + R_i + S_i&\end{aligned} \tag{4-16}$$

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 4-12.

When using the nonconservative formulation, which is the default, the fluid is assumed incompressible and divergence free: $\nabla \cdot \mathbf{u} = 0$. The nonconservative formulation improves the stability of systems coupled to a momentum equation (fluid flow equation).

To switch between the two formulations, click the **Show** button ( ) and select **Advanced Physics Options**. In the section **Advanced Settings** select either **Nonconservative form** (the default) or **Conservative form**. The conservative formulation should be used for compressible flow.

## Diffusion in Porous Media

The effective diffusion in porous media, $D_e$, depends on the structure of the porous material and the phases involved. Depending on the transport of diluted species occurs in free flow, saturated or partially saturated porous media, the effective diffusivity is defined as:

$$\begin{aligned}
D_e &= D_F && \text{Free Flow} \\
D_e &= \frac{\varepsilon_p}{\tau_L} D_L && \text{Saturated Porous Media} \\
D_e &= \frac{\theta}{\tau_L} D_L && \text{Partially Saturated Porous Media} \\
D_e &= \frac{\theta}{\tau_L} D_L + \frac{a_v}{\tau_G} k_G D_G && \text{Partially Saturated  with Volatilization}
\end{aligned}$$

Here $D_F$, $D_L$, and $D_G$ are the single-phase diffusion coefficients for the species diluted in fluid, pure liquid and gas phases 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. 12):

$$\tau_L = \theta^{-7/3} \varepsilon^2 \text{ , } \tau_G = a_v^{-7/3} \varepsilon^2$$

and Bruggeman model

$$\tau_L = \theta^{-5/2} \varepsilon^2 \text{ , } \tau_G = a_v^{-5/2} \varepsilon^2$$

For saturated porous media $\theta = \varepsilon_p$. The fluid tortuosity for the Millington and Quirk model is

$$\tau_L = \varepsilon_p^{-1/3}$$

and for the Bruggeman model the tortuosity is defined as

$$\tau_L = \varepsilon_p^{-1/2}$$

User defined expressions for the tortuosity factor can also be applied.

## *Dispersion*

The contribution of dispersion to the mixing of species typically overshadows the contribution from molecular diffusion, except when the fluid velocity is very small.

The spreading of mass, as species travel through a porous medium is caused by several contributing effects. Local variations in fluid velocity lead to mechanical mixing referred to as dispersion occurs because the fluid in the pore space flows around solid particles, so the velocity field varies within pore channels. The spreading in the direction parallel to the flow, or *longitudinal dispersivity*, typically exceeds the *transverse dispersivity* from up to an order of magnitude. Being driven by the concentration gradient alone, molecular diffusion is small relative to the mechanical dispersion, except at very low fluid velocities.

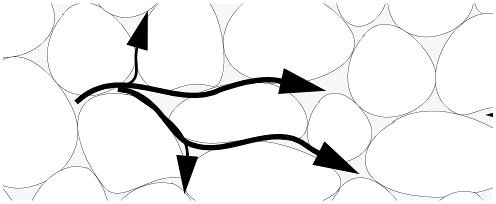

*Figure 4-2: Spreading of fluid around solid particles in a porous medium.*

is controlled through the dispersion tensor $D_D$. The tensor components can either be given by user-defined values or expressions, or derived from the directional dispersivities.

Using the longitudinal and transverse dispersivities in 2D, the dispersivity tensor components are (Ref. 9):

$$D_{\mathrm{D}ii} = \alpha_{\mathrm{L}}\frac{u_i^2}{|\mathbf{u}|} + \alpha_{\mathrm{T}}\frac{u_j^2}{|\mathbf{u}|}$$

$$D_{\mathrm{D}ij} = D_{\mathrm{D}ji} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}})\frac{u_i u_j}{|\mathbf{u}|}$$

In these equations, $D_{\mathrm{D}ii}$ (SI unit: $\mathrm{m}^2/\mathrm{s}$) are the principal components of the dispersivity tensor, and $D_{\mathrm{D}ji}$ and $D_{\mathrm{D}ji}$ are the cross terms. The parameters $\alpha_{\mathrm{L}}$ and $\alpha_{\mathrm{T}}$ (SI unit: m) specify the longitudinal and transverse dispersivities; and $u_i$ (SI unit: m/s) stands for the velocity field components.

In order to facilitate modeling of stratified porous media in 3D, the tensor formulation by Burnett and Frind (Ref. 10) can be used. Consider a transverse isotropic media, where the strata are piled up in the z direction, the dispersivity tensor components are:

$$\begin{aligned}
D_{\mathrm{L}xx} &= \alpha_1\frac{u^2}{|\mathbf{u}|} + \alpha_2\frac{v^2}{|\mathbf{u}|} + \alpha_3\frac{w^2}{|\mathbf{u}|}\\
D_{\mathrm{L}yy} &= \alpha_1\frac{v^2}{|\mathbf{u}|} + \alpha_2\frac{u^2}{|\mathbf{u}|} + \alpha_3\frac{w^2}{|\mathbf{u}|}\\
D_{\mathrm{L}zz} &= \alpha_1\frac{w^2}{|\mathbf{u}|} + \alpha_3\frac{u^2}{|\mathbf{u}|} + \alpha_3\frac{v^2}{|\mathbf{u}|}\\
D_{\mathrm{L}xy} &= D_{\mathrm{L}yx} = (\alpha_1 - \alpha_2)\frac{uv}{|\mathbf{u}|}\\
D_{\mathrm{L}xz} &= D_{\mathrm{L}zx} = (\alpha_1 - \alpha_3)\frac{uw}{|\mathbf{u}|}\\
D_{\mathrm{L}yz} &= D_{\mathrm{L}zy} = (\alpha_1 - \alpha_3)\frac{vw}{|\mathbf{u}|}
\end{aligned} \qquad (4\text{-}17)$$

In Equation 4-17 the fluid velocities $u$, $v$, and $w$ correspond to the components of the velocity field $\mathbf{u}$ in the $x$, $y$, and $z$ directions, respectively, and $\alpha_1$ (SI unit: m) is the longitudinal dispersivity. If $z$ is the vertical axis, $\alpha_2$ and $\alpha_3$ are the dispersivities in the transverse horizontal and transverse vertical directions, respectively (SI unit: m). Setting $\alpha_2 = \alpha_3$ gives the expressions for isotropic media shown in Bear (Ref. 9 and Ref. 11).

## *Adsorption*

As species travel through a porous medium they typically attach to (adsorb), and detach (desorb) from the solid phase, which slows chemical transport through the porous medium. Adsorption and desorption respectively reduces or increases species concentrations in the fluid. The adsorption properties vary between chemicals, so a plume containing multiple species can separate into components (Ref. 6). The Adsorption feature includes three predefined relationships to predict the solid concentrations, $c_{\mathrm{P}i}$ from the concentration in the liquid phase, $c_i$:

$$\begin{array}{llll} c_{\mathrm{P}} = K_P c & k_{\mathrm{P}} = \dfrac{\partial c_{\mathrm{P}}}{\partial c} = K_P & \text{User defined} & \\ c_{\mathrm{P}} = K_{\mathrm{F}}\left(\dfrac{c}{c_{\mathrm{ref}}}\right)^N & k_{\mathrm{P}} = \dfrac{\partial c_{\mathrm{P}}}{\partial c} = N\dfrac{c_{\mathrm{P}}}{c} & \text{Freundlich} & (4\text{-}18) \\ c_{\mathrm{P}} = c_{\mathrm{Pmax}}\dfrac{K_{\mathrm{L}}c}{1+K_{\mathrm{L}}c} & k_{\mathrm{P}} = \dfrac{\partial c_{\mathrm{P}}}{\partial c} = \dfrac{K_{\mathrm{L}}c_{\mathrm{Pmax}}}{(1+K_{\mathrm{L}}c)^2} & \text{Langmuir} & \end{array}$$

The above equations contains the following parameters:

- User defined isotherm $K_{\mathrm{P}}$ (SI unit: $\mathrm{m}^3/\mathrm{kg}$).
- Freundlich: Freundlich constant $K_{\mathrm{F}}$ (SI unit:·mol/kg), Freundlich exponent $N_{\mathrm{F}}$ (dimensionless), and reference concentration $c_{\mathrm{ref}}$ (SI unit: $\mathrm{mol/m}^3$).
- Langmuir: Langmuir constant $K_{\mathrm{L}}$ (SI unit: $\mathrm{m}^3/\mathrm{mol}$), and adsorption maximum $c_{\mathrm{Pmax}}$ (SI unit: mol/kg).
- These predefined expressions are adsorption isotherms that describe the amount of species sorbed to the solid. Defined at equilibrium, the switch between liquid and solid phases is instantaneous.

Using a Species Source feature, arbitrary expressions can be entered to define, for example, nonequilibrium and temperature-dependent adsorption laws, including those set out by Fetter (Ref. 7) and Bear and Verruijt (Ref. 8).

The retardation factor, RF, describes how adsorption slows the solute velocity, $\mathbf{u}_{\mathrm{c}}$, relative to the average linear velocity of the fluid, $\mathbf{u}_{\mathrm{a}}$, as in

$$\mathrm{RF} = 1 + \frac{\rho_{\mathrm{b}}}{\theta}\frac{\partial c_{\mathrm{P}}}{\partial c} = \frac{\mathbf{u}_{\mathrm{a}}}{\mathbf{u}_{\mathrm{c}}}$$

If the contaminant moves at the average linear velocity of the fluid for $\mathrm{RF} = 1$. For $\mathrm{RF} > 1$, the contaminant velocity is smaller than the fluid velocity owing to residence time on solids.

### *Reactions*

Chemical reactions of all types influence species transport in porous media. Examples include biodegradation, radioactive decay, transformation to tracked products, temperature- and pressure-dependent functions, exothermic reactions, and endothermic reactions. The reactions represent change in species concentration per unit volume porous medium per time. Reaction terms are used on the right-hand side of the governing equation to represent these processes. For reactions in a fluid phase, multiply the expression by the fluid volume fraction $\theta$. Similarly, solid phase reaction expressions include the bulk density, $\rho_\mathrm{b}$, and gas phase reactions include the gas volume fraction, $a_\mathrm{v}$.

The following expressions define some common types of reactions:

| | |
|---|---|
| $R_{Li} = -\theta\dfrac{\ln 2}{\lambda_{Li}}c_i$ | Radioactive decay — liquid |
| $R_{Pi} = -\rho_\mathrm{b}\dfrac{\ln 2}{\lambda_{Pi}}\left(\dfrac{\partial c_{Pi}}{\partial c_i}\right)c_i$ | Radioactive decay — solid |
| $R_{\mathrm{G}i} = -\dfrac{\ln 2}{\lambda_{Gi}}a_\mathrm{v}\left(\dfrac{\partial c_{\mathrm{G}i}}{\partial c}\right)c_i$ | Radioactive decay — gas |
| $R_{Lk} = \theta\zeta_{Li}c_i$ | Creation from parent $c_{Li}$ — liquid |
| $R_{Pk} = \rho_\mathrm{b}\zeta_{Pi}\left(\dfrac{\partial c_{Pi}}{\partial c_i}\right)c_i$ | Creation from sorbed parent $c_{Pi}$ — solid |
| $R_{\mathrm{G}k} = -\zeta a_\mathrm{v}\left(\dfrac{\partial c_{\mathrm{G}i}}{\partial c}\right)c_i$ | Reaction — gas |

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. 13:

$$\zeta_T = \zeta_R \exp\left[\frac{E_a(T - T_R)}{R_u T T_R}\right] \tag{4-19}$$

In Equation 4-19, $T$ 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):

$$\mathbf{u} = \frac{\kappa}{\mu}\nabla_{\mathrm{t}} p$$

Here $\mathbf{u}$ 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 4-12. The resulting equation is:

$$d_{\mathrm{fr}}\left(\frac{\partial \rho_{\mathrm{b}} c_{\mathrm{P},\,i}}{\partial t} + \frac{\partial \varepsilon_{\mathrm{p}} c_i}{\partial t} + \nabla_{\mathrm{t}} \cdot (D_{\mathrm{e},\,i} \nabla_{\mathrm{t}} c_i) + \mathbf{u} \cdot \nabla_{\mathrm{t}} c_i\right) = d_{\mathrm{fr}} R_i + d_{\mathrm{fr}} S_i + n_0 \qquad (4\text{-}20)$$

Here $d_{\mathrm{fr}}$ is the fracture thickness, $c_{\mathrm{P},\,i}$ the amount of species adsorbed to (or desorbed from) the porous matrix (moles per unit dry weight of the solid), $\varepsilon_{\mathrm{p}}$ is the fracture porosity, and $D_{\mathrm{e}}$ 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:

$$\nabla c_i = \nabla_{\mathrm{n}} c_i + \nabla_{\mathrm{t}} c_i$$

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:

$$\nabla c_i = \nabla_{\mathrm{t}} c_i$$

Using The Transport of Diluted Species in Fractures Interface, the transport along fracture boundaries alone is solved for. In this case the transport in the surrounding porous media neglected and the out-of plane flux $n_0$ vanishes.

See Fracture for more information about the boundary feature solving Equation 4-20. 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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# 5

# 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®, any description of heat transfer can be directly coupled to any other physical process. This is particularly relevant for systems based on chemical reactions and mass transfer along with fluid flow. These physics interfaces are found under the **Heat Transfer** branch ( ≋ ) when adding a physics interface.

In this chapter:

- The Mechanisms for Heat Transfer

The documentation of all features in the Heat Transfer and Heat Transfer in Porous Media interfaces are available in the *Heat Transfer Module User's Guide*, specifically in these sections:

- The Heat Transfer Module Interfaces
- The Heat Transfer in Porous Media Interface
- Theory for the Heat Transfer Module
- Theory for Heat Transfer in Porous Media

# The Mechanisms for Heat Transfer

This section includes these topics:

- Selecting the Right Heat Transfer Interface
- Heat Conduction
- Heat Convection and Conduction

- The Heat Transfer Module Interfaces
- Theory for the Heat Transfer Module
- The Heat Transfer in Porous Media Interface
- Theory for Heat Transfer in Porous Media

## *Selecting the Right Heat Transfer Interface*

The Heat Transfer branch included with the Subsurface Flow Module license includes a number of subbranches to describe energy transport.

Heat transfer through conduction and convection (both non-isothermal flow and conjugate heat transfer) in solid and free media is supported by physics interfaces shipped with the basic COMSOL Multiphysics license.

If you are using this module with enhanced Heat Transfer interface features, see also the Heat Transfer Module documentation for additional information. See Where Do I Access the Documentation and Application Libraries?

This module also includes The Heat Transfer in Porous Media Interface. The physics interface itself supports heat transfer in porous media where the thermal conductivity and heat capacity are affected by the extent of porosity. As a porous media is made up of a solid matrix filled with a fluid, heat is transported at different rates through the two types of media. The Heat Transfer in Porous Media interface provides tools and support for defining an appropriate matrix model.

The Heat Transfer in Porous Media interface characterizes temperature distributions for geological phenomena and freely couple to other features in a model. The physics interface applies to systems consisting of porous media, solids and fluids. Included are physics interfaces to calculate effective properties for porous media consisting of fluids and solid components, or a rock formation with different mineral proportions. The physics interface also features predefined expressions to represent the geotherm as a radiogenic heat source.

## *Heat Conduction*

The Heat Transfer interface in this module provides tools for analyzing heat transfer that is proportional to a temperature gradient, or conduction. It accounts explicitly for the geotherm as a heat source. This physics interface provides options to calculate thermal properties for multicomponent media. It incorporates boundary and source options to represent transversal fluxes such as convection and radiation at adjacent domains that you do not explicitly model.

The physics interface describes heat flow with negligible impacts of moving fluids. Just a few targets for conduction modeling include resistive heating in cores, estimating a surface heat flux, describing a temperature profile with depth, phase changes, exothermic reactions, and cooling earth analyses. The physics interface provides tools to consider radiative and convection heat transfers at boundaries so that you can focus on the physics in the domain of interest. With the COMSOL Multiphysics "just-type-it-in" modeling flexibility, it is straightforward to create nonlinear expressions where, for example, thermal conductivity varies with temperature as well as other physics.

Heat conduction figures into radiogenic decay, pressure-temperature phase changes, cooling-earth models, radiation, exothermic and endothermic reactions of solutes, microbial processes, diurnal heating, and many other earth processes. Conductive heat transfer can be long-term steady or exquisitely sensitive over tiny time increments. It can involve molten materials, mineral grains, fluids trapped within interstices, human-made structures, and molten rock. The heat conduction can operate within closed systems, but the geometry of interest often interacts at edges and surfaces with adjacent domains through moving fluids, conduction across a semi-insulating layer, and radiation. The models can cover such large distances that the tiny amount of heat given off by the spontaneous decay of the radiogenic particles present in most rocks produces the discernible temperature gradient with depth known to many as the geotherm.

## *Heat Convection and Conduction*

The Heat Transfer in Porous Media Interface can also set up analyses for heat transferred by convection and conduction for subsurface flow applications. Use this physics interface to describe heat carried by moving oil, water, or magma that you describe with a velocity field. Presumably the fluid velocity is nonzero but not necessarily so. You can couple the Heat Transfer interface to a Fluid Flow interface if you want to model, for example, rising magma, hot springs, liquid-steam transfers, conduction in a solid rock, buoyancy flow in streams, magma convection, and hot oil moving through a pipe. For models involving large depth changes, this physics interface provides a number of options to characterize the geothermal gradient.

The physics interface assumes that the model domain includes a single fluid moving through a domain with a number of immobile constituents, including several different solids and trapped fluids. Such is the case in many porous media.

The physics interface can also describe heat transferred with a moving fluid, which can be a surface flow or one confined to interstices in a porous medium. Analyses can cover thermal pollution migrating in a stream, transfer of hot oil into and up a well, steam injection, and diurnal heating in variably saturated soil.

This physics interface easily combines with others for an unlimited number of interesting analyses. Consider, for example, that it is straightforward to include the impacts of temperature change on hydraulic conductivity, biodegradation and chemical reaction rates, electric and magnetic potential fields, and rock strength. Likewise, you can feed back results of other physics, including reactions that consume heat, to a heat transfer model.

A variety of modeling techniques are discussed in the following sections of the *Heat Transfer Module User's Guide*:

- Heat Transfer Variables
- Using the Boundary Conditions for the Heat Transfer Interfaces
- Handling Frames in Heat Transfer
- Heat Transfer 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.

# 6

# Structural Mechanics Interfaces

This chapter describes the Poroelasticity multiphysics interface found under the **Structural Mechanics** branch ( ) when adding a physics interface. This multiphysics interface combines Darcy's law and Solid Mechanics interfaces.

In this chapter:

- The Poroelasticity Interface
- Theory for the Poroelasticity Interface

See The Solid Mechanics Interface in the *COMSOL Multiphysics Reference Manual* for details about this physics interface and feature node settings.

# The Poroelasticity Interface

The **Poroelasticity** interface ( ) combines a transient formulation of Darcy's law with a quasi-static 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 for the Darcy's Law interface.

When a predefined **Poroelasticity** interface is added from the **Structural Mechanics** branch ( ) of the **Model Wizard** or **Add Physics** windows, **Solid Mechanics** and **Darcy's Law** interfaces are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the **Poroelasticity** multiphysics coupling.

### *On the Constituent Physics Interfaces*

The Solid Mechanics interface is intended for general structural analysis of 3D, 2D, or axisymmetric bodies. In 2D, plane stress or plane strain assumptions can be used. The Solid Mechanics interface is based on solving Navier's equations, and results such as displacements, stresses, and strains are computed.

The Darcy's Law interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

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In previous versions of COMSOL Multiphysics, a specific physics interface called Poroelasticity was added to the Model Builder. Now, a predefined multiphysics coupling approach is used, improving the flexibility and design options for your modeling. For specific details, see The Multiphysics Branch and Multiphysics Modeling Approaches in the *COMSOL Multiphysics Reference Manual*.

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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.

### SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Poroelasticity**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Solid Mechanics** and **Darcy's Law** interfaces are added, an empty **Multiphysics** node appears in the model tree. You can choose from the available coupling features but the settings in the constituent interfaces are nor modified.

Coupling features are available from the context menu (right-click the **Multiphysics** node) or from the **Physics** toolbar, **Multiphysics** menu.

TABLE 6-1: 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 **Quasi-static.** |
| Darcy's Law | For the Darcy's Law interface, under Discretization, the shape function order for the temperature is set to **Linear**. Also, a **Poroelastic Storage** model is added by default. |
| Poroelasticity | The **Domain Selection** is the same as that of the participating physics interfaces.<br>The corresponding Solid Mechanics and Darcy's Law interfaces are preselected in the Coupled Interfaces section. |

*Failure of a Multilateral Well*: Application Library path **Subsurface_Flow_Module/Flow_and_Solid_Deformation/multilateral_well**

## *Poroelasticity (Multiphysics Coupling)*

The **Poroelasticity** multiphysics coupling node ( ) links bidirectionally the Solid Mechanics and Darcy's Law interfaces to account for poroelastic deformation.

### SETTINGS

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

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

The default **Name** (for the first multiphysics coupling feature in the model) is `porol`.

### DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the poroelasticity coupling, or select **All domains** as needed.

When **Poroelasticity** is added as an effect of adding a Poroelasticity interface, the selection is the same as for the participating physics interfaces.

Only domains that are active in the physics interfaces selected in the Coupled Interfaces section can be selected.

### POROELASTIC COUPLING PROPERTIES

In the **Reference pressure level** field, enter a reference pressure $p_{\mathrm{ref}}$ (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 $\alpha_{\mathrm{B}}$ (dimensionless) in the text field.

### COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Solid mechanics** and **Flow in porous media** lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (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 Poroelasticity node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Darcy's Law** is deleted, then the **Flow in porous media** list defaults to **None** as there is nothing to couple to.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Solid mechanics** or **Flow in porous media** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Approaches in the *COMSOL Multiphysics Reference Manual*.

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# Theory for the Poroelasticity Interface

The Poroelasticity Interface theory is described in this section:

- Background and Theory: Constitutive Relations
- Fluid Flow — Darcy's Law
- Solids Deformation
- Reference for the Poroelasticity Interface

## *Background and Theory: Constitutive Relations*

Poroelasticity typically describes the linked interaction between fluid flow and deformation in elastic porous media.

Of the two constitutive relations governing poroelastic behavior, one relates the stress, strain, and pore pressure:

$$\sigma = \mathbf{C}\varepsilon - \alpha_{\mathrm{B}} p_{\mathrm{f}}\mathbf{I} \qquad (6\text{-}1)$$

Here, $\sigma$ is the Cauchy stress tensor, $\varepsilon$ is the strain tensor, $\alpha_{\mathrm{B}}$ is the *Biot-Willis coefficient*, and $p_{\mathrm{f}}$ is the fluid pore pressure. The elasticity matrix $\mathbf{C}$ must in this formulation be measured under "drained" conditions, by measuring the strain induced by a change in stress under constant pore pressure.

Splitting the above relation in a volumetric and a deviatoric part, it can be seen that the deviatoric part (shear stresses) is independent of the pore pressure coupling. For an isotropic linear elastic material this means

$$\mathrm{dev}(\sigma) = 2G_{\mathrm{d}}\mathrm{dev}(\varepsilon)$$

where $G_{\mathrm{d}}$ is the shear modulus of the drained porous matrix.

The coupling in the volumetric (spherical) part can be written as

$$p_{\mathrm{m}} = -K_{\mathrm{d}}\varepsilon_{\mathrm{vol}} + \alpha_{\mathrm{B}} p_{\mathrm{f}}$$

where $K_{\mathrm{d}}$ is the bulk modulus of the drained porous matrix and

$$p_{\mathrm{m}} = -\mathrm{trace}(\sigma)/3$$

is the mean pressure (positive in compression) calculated from the stress tensor $\sigma$. The trace of the strain tensor, the volumetric strain $\varepsilon_{\mathrm{vol}}$, is a measurement of the porous matrix dilation or contraction.

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Note that the Poroelasticity multiphysics coupling adds the load from the pore pressure, $\alpha_{\mathrm{B}} p_{\mathrm{f}}$, to the Solid Mechanics interface. In this setting, the stress tensor components and mean pressure are effective stress measures.

The mean pressure is available from the Solid Mechanics interface in the variable `solid.pm` and the volumetric strain in the variable `solid.evol`. The fluid pore pressure is available from the Darcy's Law interface in the dependent variable `p`.

---

In Biot's theory (Ref. 1), the other constitutive relation relates the increment in fluid content $\zeta$ to volumetric strain and incremental pore pressure. The fluid pore pressure is proportional to the dilation of the porous matrix and the variation of fluid content:

$$p_{\mathrm{f}} = M(\zeta - \alpha_{\mathrm{B}} \varepsilon_{\mathrm{vol}}) \tag{6-2}$$

Biot and Willis (Ref. 1) measured the coefficients $\alpha_{\mathrm{B}}$ 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 $S$. It is defined through Equation 6-2 under constant volumetric strain:

$$S = \frac{1}{M} = \left.\frac{\partial \zeta}{\partial p_{\mathrm{f}}}\right|_{\varepsilon_{ii}}$$

Using this definition, it is possible to measure the storage coefficient directly in the lab, but at least in the case of an ideal porous material it can be calculated from basic material properties as

$$S = \frac{\varepsilon_{\mathrm{p}}}{K_{\mathrm{f}}} + \frac{\alpha_{\mathrm{B}} - \varepsilon_{\mathrm{p}}}{K_{\mathrm{s}}} \tag{6-3}$$

Here, $\varepsilon_{\mathrm{p}}$ is the porosity, $K_{\mathrm{f}}$ the fluid bulk modulus (the inverse of the fluid compressibility $\chi_{\mathrm{f}}$), and $K_{\mathrm{s}}$ the solid bulk modulus (that is, the would-be bulk modulus of a homogeneous block of the solid material making up the porous matrix).

The parameter $\alpha_B$ is the Biot-Willis coefficient, which relates the volume of fluid expelled (or sucked into) a porous material element to the volumetric change of the same element.

The Biot-Willis coefficient can be measured experimentally or defined in terms of the drained and solid bulk moduli as

$$\alpha_B = \left.\frac{\partial p_m}{\partial p_f}\right|_{\varepsilon_{ii}} = 1 - \frac{K_d}{K_s}$$

The drained bulk modulus $K_d$ is always smaller than the solid bulk modulus $K_s$ (a solid block is stiffer than a porous block made of the same material), and therefore the Biot-Willis coefficient is always bounded to $\varepsilon_p \le \alpha_B \le 1$.

The parameter $\alpha_B$ does not depend on the properties of the fluid, but on the properties of the porous matrix. A soft porous matrix has a Biot-Willis coefficient close to 1 (since $K_d << K_s$), while for a stiff matrix, it is close to the porosity (since $K_d \approx (1-\varepsilon_p)K_s$)

Using the expression for the parameter $\alpha_B$, the storage coefficient $S$ is calculated in terms of the porosity $\varepsilon_p$, Biot-Willis coefficient $\alpha_B$, and the bulk moduli of the fluid $K_f$ and drained porous matrix $K_d$

$$S = \frac{\varepsilon_p}{K_f} + (\alpha_B - \varepsilon_p)\frac{1-\alpha_B}{K_d} \tag{6-4}$$

## *Fluid Flow — Darcy's Law*

Darcy's law describes the flow field in the poroelastic model. The fluid equation comes from the mass conservation

$$\frac{\partial}{\partial t}(\rho_f \varepsilon_p) + \nabla \cdot (\rho_f \mathbf{u}) = Q_m \tag{6-5}$$

Darcy's velocity including gravity reads

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p_f + \rho_f g \nabla D)$$

and the storage model

$$\frac{\partial}{\partial t}(\rho_f \varepsilon_p) = \rho_f S \frac{\partial p_f}{\partial t}$$

which translates the mass conservation equation to

$$\rho_f S \frac{\partial p_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}) = -\rho_f \alpha_B \frac{\partial}{\partial t} \varepsilon_{\mathrm{vol}} \qquad (6\text{-}6)$$

here, $\partial\varepsilon_{\mathrm{vol}}/\partial t$ 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. The poroelastic storage term $S$ is calculated from Equation 6-4.

You can interpret the right-hand term as the rate of expansion of the pore space. As $\partial\varepsilon_{\mathrm{vol}}/\partial t$ increases, the volume fraction available for the fluid also increases and thereby gives rise to liquid sink, therefore the negative sign in the source term $Q_m = -\rho_f \alpha_B \partial\varepsilon_{\mathrm{vol}}/\partial t$.

## *Solids Deformation*

Navier's equations for a solid in equilibrium under purely gravitational load is

$$-\nabla \cdot \sigma = \rho_{\mathrm{av}} \mathbf{g} = (\rho_f \varepsilon_p + \rho_d) \mathbf{g} \qquad (6\text{-}7)$$

where $\sigma$ is the total stress tensor from Equation 6-1 and $\rho_{\mathrm{av}}$, $\rho_f$, and $\rho_d$ represent average, fluid, and drained densities, respectively, and $\varepsilon_p$ is the porosity. The fluid-to-structure coupling therefore enters as an additional isotropic term in the stress tensor, which, in analogy with general initial stresses, can be identified as an initial pressure.

Equation 6-7, 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 because the time scale of the structural response is generally many orders of magnitude faster than the time scale of the flow. When you study the coupled process on the time scale of the flow, you can therefore assume that the solid reaches a new equilibrium immediately in response to a change in the flow conditions. This means that the stresses and strains change in time — even if Equation 6-7 appears to be stationary — and that the structure-to-fluid coupling term, involving the rate of strain, is nonzero.

## *Reference for the Poroelasticity Interface*

1. M.A. Biot, "Mechanics of Deformation and Acoustic Propagation in Porous Media", *J. Appl. Phys.*, vol. 33, pp. 1482–1498, 1962.

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