COMSOL MULTIPHYSICS

EARTH SCIENCE MODULE

USER'S GUIDE

VERSION 3.5a

COMSOL

How to contact COMSOL:

Benelux
COMSOL BV
Röntgenlaan 19
2719 DX Zoetermeer
The Netherlands
Phone: +31 (0) 79 363 4230
Fax: +31 (0) 79 361 4212
info@comsol.nl
www.comsol.nl

Denmark
COMSOL A/S
Diplomvej 376
2800 Kgs. Lyngby
Phone: +45 88 70 82 00
Fax: +45 88 70 80 90
info@comsol.dk
www.comsol.dk

Finland
COMSOL OY
Arabianranta 6
FIN-00560 Helsinki
Phone: +358 9 2510 400
Fax: +358 9 2510 4010
info@comsol.fi
www.comsol.fi

France
COMSOL France
WTC, 5 pl. Robert Schuman
F-38000 Grenoble
Phone: +33 (0)4 76 46 49 01
Fax: +33 (0)4 76 46 07 42
info@comsol.fr
www.comsol.fr

Germany
COMSOL Multiphysics GmbH
Berliner Str. 4
D-37073 Göttingen
Phone: +49-551-99721-0
Fax: +49-551-99721-29
info@comsol.de
www.comsol.de

Italy
COMSOL S.r.l.
Via Vittorio Emanuele II, 22
25122 Brescia
Phone: +39-030-3793800
Fax: +39-030-3793899
info.it@comsol.com
www.it.comsol.com

Norway
COMSOL AS
Søndre gate 7
NO-7485 Trondheim
Phone: +47 73 84 24 00
Fax: +47 73 84 24 01
info@comsol.no
www.comsol.no

Sweden
COMSOL AB
Tegnérgatan 23
SE-111 40 Stockholm
Phone: +46 8 412 95 00
Fax: +46 8 412 95 10
info@comsol.se
www.comsol.se

Switzerland
FEMLAB GmbH
Technoparkstrasse 1
CH-8005 Zürich
Phone: +41 (0)44 445 2140
Fax: +41 (0)44 445 2141
info@femlab.ch
www.femlab.ch

United Kingdom
COMSOL Ltd.
UH Innovation Centre
College Lane
Hatfield
Hertfordshire AL10 9AB
Phone:+44-(0)-1707 636020
Fax: +44-(0)-1707 284746
info.uk@comsol.com
www.uk.comsol.com

United States
COMSOL, Inc.
1 New England Executive Park
Suite 350
Burlington, MA 01803
Phone: +1-781-273-3322
Fax: +1-781-273-6603

COMSOL, Inc.
10850 Wilshire Boulevard
Suite 800
Los Angeles, CA 90024
Phone: +1-310-441-4800
Fax: +1-310-441-0868

COMSOL, Inc.
744 Cowper Street
Palo Alto, CA 94301
Phone: +1-650-324-9935
Fax: +1-650-324-9936

info@comsol.com
www.comsol.com

For a complete list of international representatives, visit www.comsol.com/contact

Company home page
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Introduction

The Earth Science Module is an optional package that extends the COMSOL Multiphysics® modeling environment to the quantitative investigation of geophysical and environmental phenomena. It is designed for researchers, engineers, developers, teachers, and students, and it suits both single-physics and interdisciplinary study. The earth and planets make up 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 contents of the Earth Science Module are a set of fundamental building blocks with which to pose and answer a wide array of physics questions. The equation interfaces it offers function on their own and link arbitrarily. They also couple to physics already built into COMSOL Multiphysics, to any new equations you create, and to the application modes in the other specialized modules. Because COMSOL Multiphysics removes the complications of writing your own code, it is our hope that you will use the Earth Science Module as a springboard to learn and to explore a rich variety of physics modeling.

The Earth Science Module includes equation interfaces (which we call application modes) geared to earth-science investigations as well as a bank of worked example models that address an interesting range of problems. To the best of our knowledge, the equations represented here are not collected in any other single software package. The ready-to-run models we chose for the library demonstrate a range of the features included in the module and also provide insight into COMSOL Multiphysics modeling in general. Each model comes with step-by-step instructions to reproduce it in the graphical user interface along with any data or additional files needed to build it on your own. Those who are unfamiliar with some of the equations or computational techniques included in the module should find the models and the documentation extremely beneficial.

We have tailored the interfaces, options, and functionalities in this module especially to account for geologic process terms. The heat transfer application modes, for example, feature interfaces to superpose a background geotherm without incorporating it as a boundary condition. These application modes also include options to automate the calculation of effective thermal properties for multicomponent systems. The fluid-flow equations represent a wide range of possibilities. Included are Richards' equation, which describes nonlinear flow in variably saturated porous media. The options for saturated porous media include Darcy's law for slow flow and the Brinkman equations where shear is non-negligible. The Navier-Stokes equations cover free flows. The module also treats the transport of chemicals and their reactions. The Solute Transport application modes account for chemical transfer in solid, liquid, and gas phases for free, saturated, and variably saturated fluid flows. A number of the examples in the model library link these application modes together. Some also bring in other physics from COMSOL Multiphysics.

The documentation set for the Earth Science Module consists of two books. This volume, the *Earth Science Module User's Guide*, introduces the basic modeling process. It includes chapters presenting the different application modes available in the module and discussing the modeling strategy for various test cases. The final chapter details the application modes and how COMSOL Multiphysics implements them.

The second book in the set, the *Earth Science Module Model Library*, opens with a straightforward but innovative example "Pore-Scale Flow" that describes free flow with the Navier-Stokes equations within the microscale interstices of a rock slice. The library then works through other fluid-flow examples and proceeds with models of fluid flow coupled to other physical processes including solid-deformation, solute transport and heat transfer. It also contains additional multiphysics models such as electrokinetic flow in a volcano. The authors obtained a number of these state-of-the-art examples from researchers using COMSOL Multiphysics in their work. Others are reproductions from cases in international scientific journals. Each model comes with theoretical background as well as step-by-step instructions that illustrate how to set it up. Further, we supply these models as COMSOL Multiphysics model files so you can import them into COMSOL Multiphysics for immediate access. This way you can follow along with the printed discussion as well as use them as a jumping-off point for your own modeling needs.

We hope the Earth Science Module becomes a valuable tool in your modeling work. We are convinced that the effort you put into understanding COMSOL Multiphysics will be repaid many times. If you have feedback on the module or the models in the library or if you have ideas for additional application modes or examples that we could add, we welcome your suggestions. Feel free to contact us at info@comsol.com.

New Features in the Earth Science Module 3.5a

This new release of the Earth Science Module includes a number of valuable new capabilities, including the following features:

- Predefined multiphysics interface for modeling of poroelasticity, combining Darcy's law with a structural mechanics application mode. Requires the Structural Mechanics Module or the MEMS Module. For more information, see "Poroelasticity" on page 54.
- Improved performance and stabilization for fluid-flow modeling using the Navier-Stokes and Brinkman equations.
- The Liquid and Gases material library, which contains thermal and fluid dynamics properties for a set of common fluids. For more information, see "The Liquids and Gases Library and Material Property Functions" on page 95.
- Improved Model Library with three new models:
  - Aquifer Water Table: Instead of being assumed, the shape of the water table is computed in this model to correctly model groundwater flow in an aquifer.
  - Aquifer Characterization: Estimating the hydraulic-conductivity field in an aquifer using inverse modeling and experimental data (requires the Optimization Lab).
  - Forchheimer Flow: The resistance to flow in open porous structures, like packed beds, is governed by both laminar and turbulent effects. The Forchheimer equation takes this into account.

Typographical Conventions

All COMSOL manuals use a set of consistent typographical conventions that should make it easy for you to follow the discussion, realize what you can expect to see on the screen, and know which data you must enter into various data-entry fields. In particular, you should be aware of these conventions:

- A **boldface** font of the shown size and style indicates that the given word(s) appear exactly that way on the COMSOL graphical user interface (for toolbar buttons in the corresponding tooltip). For instance, we often refer to the **Model Navigator**, which is the window that appears when you start a new modeling session in COMSOL; the corresponding window on the screen has the title **Model Navigator**. As another example, the instructions might say to click the **Multiphysics** button, and the boldface font indicates that you can expect to see a button with that exact label on the COMSOL user interface.
- The names of other items on the graphical user interface that do not have direct labels contain a leading uppercase letter. For instance, we often refer to the Draw toolbar; this vertical bar containing many icons appears on the left side of the user interface during geometry modeling. However, nowhere on the screen will you see the term “Draw” referring to this toolbar (if it were on the screen, we would print it in this manual as the **Draw** menu).
- The symbol **>** indicates a menu item or an item in a folder in the **Model Navigator**. For example, **Physics>Equation System>Subdomain Settings** is equivalent to: On the **Physics** menu, point to **Equation System** and then click **Subdomain Settings**. **COMSOL Multiphysics>Heat Transfer>Conduction** means: Open the **COMSOL Multiphysics** folder, open the **Heat Transfer** folder, and select **Conduction**.
- A `Code` (monospace) font indicates keyboard entries in the user interface. You might see an instruction such as “Type `1.25` in the **Current density** edit field.” The monospace font also indicates code.
- An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or in the Glossary. The names of books in the COMSOL documentation set also appear using an italic font.

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Overview

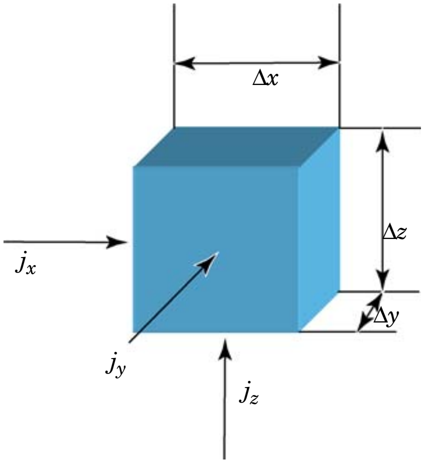
This chapter gives an overview of the application modes in the Earth Science Module. The application modes provide the modeling interfaces for the various types of physics that this module covers: fluid flow, heat transfer, and solute transport.

Modeling in the Earth Science Module

The Earth Science Module contains a set of application modes adopted for a broad category of simulations important in earth investigations. To the best of our knowledge, the equations represented here are not customarily lumped into a single package. These application modes and models can serve equally well as tools for academic research, applied investigations, and classroom education.

Numerical modeling typically begins with a question about some physical phenomenon within a particular region of interest. Defining the question well typically means the type of information needed to answer it is obvious. You then identify which physics are actually important to answering the question and how they interact. Next you define a mathematical model fitted 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, you interpret the results 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. 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



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

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 Δt. 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

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

Allowing the time period Δt and the volume to become infinitesimally small gives the base equation for a large family of problems in Earth sciences:

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

This equation appears in different forms throughout this manual and the accompanying *Earth Science Module Model Library.* 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, you must specify proper initial conditions and boundary conditions.

Application Mode Guide

The Earth Science Module contains a number of application modes that predefine equations or sets of equations adapted to earth-science applications. You can take the equations in these application modes and the variables they offer and then modify them, link them together, and couple them to physics represented elsewhere in COMSOL Multiphysics. This module handles time-dependent and stationary problems for 1D, 2D, and 3D systems with axisymmetry for 1D and 2D. The predefined physics cover three main categories:

- Fluid flow. This group of application modes estimates the pressure and velocity of fluids flowing in free systems and within the interstices of a porous medium. They include the Navier-Stokes equations for surface and other free flows; the Brinkman equations for fast flow in porous media flow; Darcy's law for flow in porous media that is relatively slow; and Richards' equation for variably saturated systems. With Darcy's law and Richards' equation, COMSOL Multiphysics solves for pressure and offers interfaces for pressure head and hydraulic head. You can set up these equations for single or multiple fluids. You can also couple them to other physics to describe poroelasticity, convection of heat and density driven flows, solute transfer, and electromagnetic forces, to name a few. For poroelasticity, the Poroelasticity predefined multiphysics coupling (requires the Structural Mechanics Module or the MEMS Module) sets up the Darcy's Law application mode together with a structural mechanics application mode and provides suitable settings for describing the interaction between the solid and the fluid.
- Heat transfer. This group of application modes estimates the temperature distribution in solids, fluids, and fluid-solid systems. It includes interfaces to estimate effective properties in multicomponent systems. All heat transfer application modes come with interfaces to account for a geotherm brought about through radiogenic decay. The Conduction application mode describes heat transfer for domains with negligible fluid movement. The Convection and Conduction application mode characterizes 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.
- Solute transport. These application modes characterize 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 advection, dispersion, diffusion, sorption, and reactions. You define the convective term in the mass-transport vector either with any of the momentum balances just mentioned or you set it to a predefined velocity profile.

The chapters that follow describe the predefined equations and boundary conditions for the application modes in the Earth Science Module. A discussion at the end of this manual details how these equations are formulated within COMSOL Multiphysics.

TABLE 2-1: APPLICATION MODES IN THE EARTH SCIENCE MODULE

APPLICATION MODES	**MODE NAME**	**DEPENDENT VARIABLE**	**1D**	**2D**	**3D**	**STATIONARY**	**TRANSIENT**
FLUID FLOW APPLICATION MODES							
Brinkman equations, Cartesian coordinates	chns	u, p		√	√	√	√
Brinkman equations, axisymmetry	chns	u, p		√		√	√
Darcy's law, Cartesian coordinates	esdl	p	√	√	√	√	√
Darcy's law, axisymmetry	esdl	p	√	√		√	√
Pressure analysis			√	√	√	√	√
Pressure head analysis			√	√	√	√	√
Hydraulic head analysis			√	√	√	√	√
Incompressible Navier-Stokes, Cartesian coordinates	chns	u, p		√	√	√	√
Incompressible Navier-Stokes, axisymmetry	chns	u, p		√		√	√
Weakly compressible Navier-Stokes				√	√	√	√
Swirl flow, axisymmetry				√			
Richards' equation, Cartesian coordinates	esvr	p	√	√		√	√
Richards' equation, axisymmetry	esvr	p	√	√		√	√
Pressure analysis			√	√	√	√	√
Pressure head analysis			√	√	√	√	√
Hydraulic head analysis			√	√	√	√	√
HEAT TRANSFER APPLICATION MODES							
Conduction, Cartesian coordinates	eshc	T	√	√	√	√	√
Conduction, axisymmetry	eshc	T	√	√	√	√	√
Solids			√	√	√	√	√

TABLE 2-1: APPLICATION MODES IN THE EARTH SCIENCE MODULE

APPLICATION MODES	**MODE NAME**	**DEPENDENT VARIABLE**	**1D**	**2D**	**3D**	**STATIONARY**	**TRANSIENT**
Porous media			√	√	√	√	√
Convection and conduction, Cartesian coordinates	eshcc	T	√	√	√	√	√
Convection and conduction, axisymmetry	eshcc	T	√	√		√	√
Mobile fluid			√	√	√	√	√
Mobile fluid/solids			√	√	√	√	√
Mobile fluid/immobile fluid/solids			√	√	√	√	√
SOLUTE TRANSPORT APPLICATION MODES							
Solute transport, Cartesian coordinates	esst	c	√	√	√	√	√
Solute transport, axisymmetry	esst	c	√	√		√	√
Non-conservative			√	√	√	√	√
Conservative			√	√	√	√	√
Liquid			√	√	√	√	√
Liquid-Solid			√	√	√	√	√
Variably saturated solute transport, Cartesian	esst	c	√	√	√	√	√
Variably saturated solute transport, axisymmetry	esst	c	√	√		√	√
Non-conservative			√	√	√	√	√
Conservative			√	√	√	√	√
Liquid			√	√	√	√	√
Liquid-Solid			√	√	√	√	√
Liquid-Solid-Gas			√	√	√	√	√

3

Fluid Flow Application Modes

This chapter provides information about the application modes for modeling fluid flow in the Earth Science Module. In addition, the final section describes the predefined multiphysics couplings for poroelasticity, which combine Darcy's law with application modes for structural equations.

Overview

The fluid flow application modes in the Earth Science Module provide tools for characterizing movements of liquids, gases, and other flowing media, such as molten rock. Four sets of equations that apply under different conditions form the basis for this application modes in this group:

- *Darcy's law* describes low-velocity flows of one or more fluids.
- For porous media, *the Brinkman equations* cover high-velocity flows.
- *Richards' equation* governs the wetting and drying of rocks or soils.
- *The Navier-Stokes equations* describe free flows within a river or well, for example.

The corresponding application modes combine arbitrarily and link to other physics including solute transport, heat transfer, electric potentials, magnetic potential, and structural deformation, to name a few. Because you can type in any expression 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.

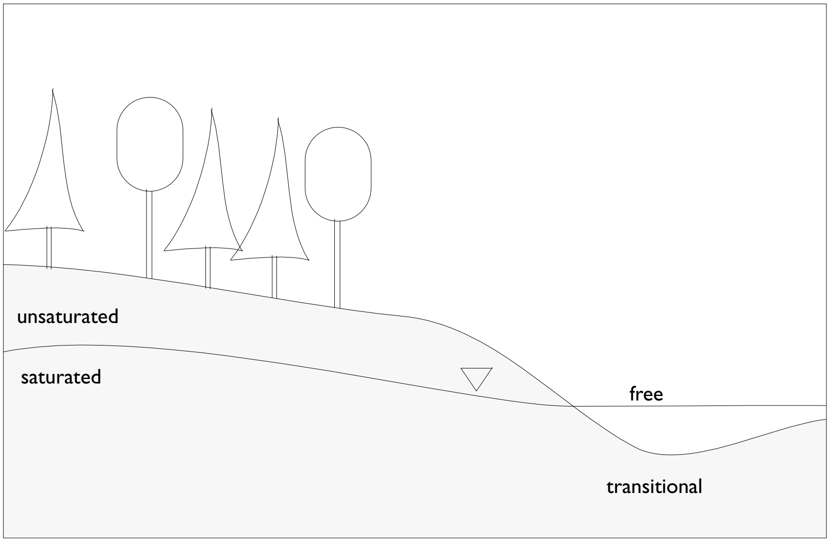


Figure 3-1: Vertical cross section through ground near a river. Labels indicate flow regimes. The triangle denotes the water table.

The Navier-Stokes equations cover 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; for example, see “Pore-Scale Flow” on page 8 of the *Earth Science Module Model Library.* 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 application modes offered here—Darcy’s law, the Brinkman equations, 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 application modes in this module can be grouped according to driving forces. Consider Bernoulli’s equation for mechanical energy along a streamline in inviscid fluids:

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

Here s represents a location on the streamline, u denotes the fluid velocity, ρ_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 Navier-Stokes equations 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 application modes.

Darcy's Law—Pressure

Subdomain Equations

The Earth Science Module's Darcy's Law application mode 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 application modes apply 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). You can also set up multiple Darcy's Law application modes to model multiphase flows involving more than one mobile phase.

Darcy's law applies when the gradient in hydraulic potential drives fluid movement in the porous medium. You can 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

$$\mathbf{u} = -\frac{\kappa}{\eta}(\nabla p + \rho_f g \nabla D) .$$

In this equation, $\mathbf{u}$ is the Darcy velocity or specific discharge vector (m/s); κ is the permeability of the porous medium (m^2); η is the fluid's dynamic viscosity (Pa·s); p is the fluid's pressure (Pa) and ρ_f is its density (kg/m^3); g is the magnitude of gravitational acceleration (m/s^2); and ∇D is a unit vector in the direction over which g acts. Here the permeability, κ, represents the resistance to flow over a representative volume consisting of many solid grains and pores.

The hydraulic potential in the equation comes from the pressure, p, and gravity, $\rho_f g D$. COMSOL Multiphysics solves for the pressure, p. You set the gravitational vector's magnitude, g, directly and its direction by specifying the coordinate, D. The choices related to gravity simplify modeling certain geometries and facilitate investigations of fluid movements on planets other than earth. By default, g equals 9.82 m/s^2 and D is zero. 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 flow is entirely horizontal within the xy-plane, then the gradient in D vanishes and the driving force is pressure gradients alone.

Inserting Darcy's law into the equation of continuity produces the generalized governing equation

$$\frac{\partial}{\partial t}(\rho_f\theta_s) + \nabla \cdot \rho_f\mathbf{u} = \rho_f Q_s$$

$$\frac{\partial}{\partial t}(\rho_f\theta_s) + \nabla \cdot \rho_f\left[-\frac{\kappa}{\eta}(\nabla p + \rho_f g\nabla D)\right] = \rho_f Q_s \tag{3-1}$$

where θ_s denotes the fluid volume fraction and Q_s is the strength of a fluid source (1/s). You can represent this equation fully in COMSOL Multiphysics because you can freely specify relationships between density or permeability, for example, and pressure, temperature, concentration, and so on.

For an incompressible fluid, ρ_f moves outside the divergence operator, and the governing equation (Equation 3-1) takes the common form shown by default in the user interface:

$$S\frac{\partial p}{\partial t} + \nabla \cdot \left[-\frac{\kappa}{\eta}(\nabla p + \rho_f g\nabla D)\right] = Q_s \tag{3-2}$$

In the equation, S is a storage coefficient (1/Pa), which can be an expression that perhaps involves results from a solid-deformation equation set up in the model or temperatures and concentrations from other analyses. COMSOL Multiphysics explicitly includes expression fields to define S as specific storage using fluids and solids compressibility data. The Darcy's Law application mode implements Equation 3-2 and assumes that the fluid is incompressible (the density ρ_f is constant).

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, we set out the average linear velocity within a given pore space, $\mathbf{u}_\alpha$, (also termed the seepage velocity) defined as $\mathbf{u}_\alpha = \mathbf{u}/\theta_s$, where θ_s is the fluid volume fraction. For saturated systems, θ_s equals the porosity.

Scaling Coefficients

In the Earth Science Module, the Darcy's law application mode provides optional scaling coefficients to facilitate advanced analyses and iterative or parametric simulations. The types of analyses that the scaling coefficients enable include dual-domain systems involving relatively fast flow in fractures, multiphase problems, and density dependencies, to name a few. With the optional coefficients, the governing equation takes the form

$$\delta_S S\frac{\partial p}{\partial t} + \nabla \cdot \left[-\delta_K \frac{\kappa}{\eta}(\nabla p + \rho_f g \nabla D)\right] = \delta_Q Q_s\,.$$

In this equation, δ represents a scaling coefficient, and the subscripts "S," "K," and "Q" denote the corresponding term in the equation.

Boundary Conditions

A unique solution to the governing statements requires boundary conditions for all models. It also requires initial conditions for transient or time-dependent problems. The Darcy's law application mode of the Earth Science Module provides a number of boundary conditions (Ref. 5). You can also freely specify unique conditions by entering expressions in the boundary settings dialog boxes or by altering the boundary mechanics in the equation systems dialog boxes.

In many cases you know the distribution of pressure giving the 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.

At a free surface, such as a spring or a seepage face, pressure is atmospheric. If you gauge the pressures in the model 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 $\rho_f g D$.

Fluid does not move across impervious boundaries. You represent this effect with the zero flux condition

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

where $\mathbf{n}$ is the vector normal to the boundary. While this Neumann condition specifies zero flow across the boundary, it allows for movement along it. In this way the equation for the zero flux condition also describes symmetry about an axis or a flow divide, for example.

Often you can determine the fluid flux from the pumping rate or from measurements. With the inward flux boundary condition, positive values correspond to flow into the model domain

$$\mathbf{n}\cdot\frac{\kappa}{\eta}(\nabla p + \rho_{\mathrm{f}} g \nabla D) = N_0$$

where N_0 (m/s) is a value or expression for the inward Darcy flux that you specify.

Occasionally you need to specify the inward flux, N_0, combined with information about the hydraulic potential at some finite distance. The model domain might connect to a larger body of water through a semi-pervious layer. You can represent this condition with the mixed boundary expression

$$\mathbf{n}\cdot\frac{\kappa}{\eta}(\nabla p + \rho_{\mathrm{f}} g \nabla D) = N_0 + R_{\mathrm{b}}[(p_{\mathrm{b}} - p) + \rho_{\mathrm{f}} g (D_{\mathrm{b}} - D)] \tag{3-3}$$

where p_{b} (Pa) and D_{b} (m) are the pressure and elevation of the distant fluid source; and R_{b} ($\mathrm{m}^2\cdot\mathrm{s/kg}$) is the "conductance" of materials between the source and the model domain. Typically $R_{\mathrm{b}} = K'/(\eta\cdot B')$, where K' is the permeability (m^2) of the thin layer and B' (m) is its thickness. Using logical relationships, it is possible to activate these expressions at different times or under various flow conditions.

References

1. J. Bear, *Hydraulics of Groundwater*, McGraw-Hill, 1979.

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Darcy's Law—Head

Introduction

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 Darcy's law application modes in the Earth Science Module provide interfaces for hydraulic head and pressure head analyses. For these analyses, COMSOL Multiphysics calculates head from the pressure solution and provides corresponding interfaces for material properties, boundary conditions, and postprocessing. In the Darcy's law application modes, pressure always is the dependent variable. You see the equations that relate pressure p to the total hydraulic head H or the pressure head H_p in the user interface.

Hydraulic head, H, pressure head, H_p, and elevation head, D, relate to pressure p as

$$\frac{p + \rho_f g D}{\rho_f g} = H = H_p + D$$

where ρ_f is fluid density, g denotes the magnitude of gravitational acceleration, 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.

Models can define capacity to transmit flow

$$\frac{\kappa}{\eta} = \frac{K}{\rho_f g}$$

using κ the intrinsic permeability of the porous medium, and η is the fluid viscosity of the fluid or hydraulic conductivity, K (m/s). The hydraulic conductivity represents both fluid and solid properties.

Subdomain Equations—Hydraulic Head Analysis

For analyses built on hydraulic head with hydraulic conductivity, the velocity $\mathbf{u}$ according to Darcy's law is

$$\mathbf{u} = -K\nabla H .$$

The governing equation becomes

$$S\frac{\partial H}{\partial t} + \nabla \cdot [-K\nabla H] = Q_s \tag{3-4}$$

where S is the storage coefficient defined for head, and Q_s is a fluid source.

The boundary conditions in the hydraulic-head interface are the mix of Dirichlet, Neumann, and Cauchy conditions described for pressure. The previous section on Darcy's law for pressure fully describes the physical meaning behind each boundary condition. The expressions are

$H = H_0$	Hydraulic head
$H = D$	Free surface
$\mathbf{n} \cdot K\nabla H = 0$	Zero flux
$\mathbf{n} \cdot K\nabla H = 0$	Symmetry
$\mathbf{n} \cdot K\nabla H = N_0$	Flux
$\mathbf{n} \cdot K\nabla H = N_0 + R_\mathrm{b}[H_\mathrm{b} - H]$	Mixed

where $\mathbf{n}$ is the normal to the boundary, H_0 is the specified hydraulic head, N_0 is a specified flux, R_b represents conductance to flow in a semi-pervious layer adjacent to the boundary, and H_b is the hydraulic head at the edge of the layer. 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.

Subdomain Equations—Pressure Head Analysis

For pressure head analyses in the Darcy's law application mode, the velocity $\mathbf{u}$ is

$$\mathbf{u} = -K\nabla(H_p + D)$$

when using hydraulic conductivity K to describe material properties.

The governing equation explicitly references the elevation head:

$$S\frac{\partial H_p}{\partial t} + \nabla \cdot [-K\nabla(H_p + D)] = Q_s .$$

Again you enter the storage coefficient, S, as defined for a dependent variable of head.

The boundary conditions shown in the pressure head interfaces are

$H_p = H_{p0}$	Pressure head
$H_p = 0$	Free surface
$\mathbf{n} \cdot K\nabla(H_p + D) = 0$	Zero flux
$\mathbf{n} \cdot K\nabla(H_p + D) = 0$	Symmetry
$\mathbf{n} \cdot K\nabla(H_p + D) = N_0$	Flux
$\mathbf{n} \cdot K\nabla(H_p + D) = N_0 + R_\mathrm{b}[(H_{p\mathrm{b}} + D_\mathrm{b}) - (H_p + D)]$	Mixed

and here the user defines the free surface by setting the pressure head, H_p, to zero.

Using Hydraulic Head and Pressure Head in Expressions

In the Darcy's Law Hydraulic Head Analysis and Pressure Head Analysis application modes you enter inputs in units of head. Because COMSOL Multiphysics translates your inputs to solve for pressure, you can use the dependent variable p and its gradients in any expression. For example, in postprocessing you can enter `p`, `px`, and `py` in an edit field to access pressure and its gradients in the x and y directions.

You use a suffix when referencing other coefficients and variables defined in the **Physics** settings of the model, including pressure head or hydraulic head. For example, the default name for a Darcy's law application from the Earth Science module is **esdl**. This name appears at the top of the COMSOL Multiphysics user interface, in the lower left corner of the Model Navigator, and in the physics settings dialog boxes. For example, you can reference hydraulic head, H, in defining material properties. In fracture zones hydraulic conductivity can decrease with hydraulic head according to $K_s = 25 - H/H_0$. Once you define H_0 as a constant or expression in the **Options** settings, or as a solution in another equation in the model, you could simply enter `25-H_esdl/H0` in the $\mathbf{K_s}$ edit field.

Note that if a model contains more than one equation in which p is the dependent variable, the software by default designates the second instance as **p2**. Likewise, the second instance of a Darcy's law application mode is **esdl2**.

You can freely inspect the solution mechanics and the different variable definitions from the **Physics>Equation System** dialog boxes. If you want to modify the equation setup, however, we encourage you to formulate the problem in the Darcy's Law Pressure Analysis application mode.

Richards' Equation—Flow in Variably Saturated Porous Media

Subdomain Equation

The Richards' Equation application mode analyzes 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 application mode 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.

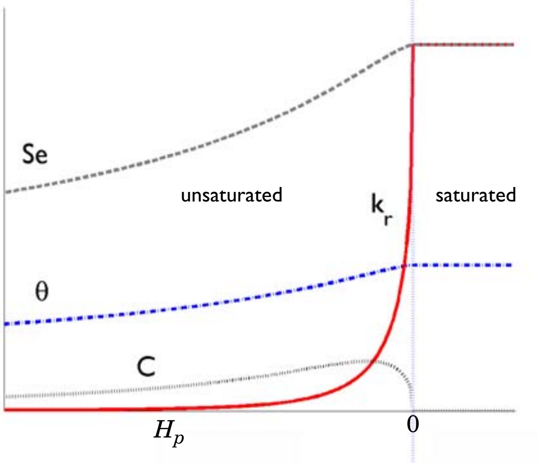

Figure 3-2: Fluid retention and permeability functions that vary with pressure head, as given by Van Genuchten formulas available in the Richards' Equation application mode.

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):

$$\delta_{\mathrm{ts}}\left[\frac{C}{\rho_{\mathrm{f}}g}+\mathrm{Se}S\right]\frac{\partial p}{\partial t}+\nabla\cdot\left[-\frac{\kappa_s}{\eta}k_{\mathrm{r}}(\nabla p+\rho_{\mathrm{f}}g\nabla D)\right] = Q_s$$

where pressure, p, is the dependent variable. In this equation, δ_{ts} is an optional time-scaling coefficient (equal to 1 by default), C represents the specific capacity, Se denotes the effective saturation, S is the storage coefficient, κ_{s} gives the intrinsic permeability, η is the fluid viscosity, k_{r} denotes the relative permeability, ρ_{f} is the fluid density, g is gravitational acceleration, D represents the vertical coordinate, and Q_s is the fluid source (positive) or sink (negative). Like Darcy's law, COMSOL Multiphysics solves the Richards' equation for a dependent variable of pressure but provides interfaces for hydraulic-head and pressure-head analyses.

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

$$\mathbf{u} = -\frac{\kappa_s}{\eta} k_{\mathrm{r}} (\nabla p + \rho_{\mathrm{f}} g \nabla D)$$

where $\mathbf{u}$ is the flux vector. The porous medium consists of voids, 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, θ. This interstitial or average linear velocity is $\mathbf{u}_{\mathrm{a}} = \mathbf{u}/\theta$.

Retention and Permeability Relationships

Richards' equation appears deceptively similar to the saturated flow equation set out in the Darcy's Law application mode, but it is notoriously nonlinear (Ref. 3). Nonlinearities arise because the material and hydraulic properties θ, Se, C, and k_{r} vary for unsaturated conditions (for example, negative pressure) and reach a constant value at saturation (for example, pressure of zero or above). The volume of liquid per porous medium volume, θ, ranges from a small residual value θ_{r} to the total porosity θ_{s}. Its value is given in a constitutive relation in the model. The effective saturation, Se, amounts to θ normalized to a maximum value of 1. The specific capacity, C, describes the change in θ as the solution progresses, the slope on a plot of θ versus pressure (or pressure head). The relative permeability, k_{r}, increases with moisture content and varies from a nominal value to 1. That k_{r} attains maximum value at saturation reveals that fluid moves more readily when the porous medium is fully wet.

The Richards' Equation application modes in COMSOL Multiphysics offer three methods to define θ, Se, C, and k_{r}. The analytic formulas of van Genuchten (Ref. 4) and Brooks and Corey (Ref. 5) are so frequently employed that they are synonymous with this variably saturated flow modeling. Posed in terms of pressure head $H_p = p/(\rho_{\mathrm{f}} g)$, the analytic expressions require data for the saturated θ_{s} and residual θ_{r} liquid volume fractions as well as constants α, n, m, and l, which specify a particular media type.

The van Genuchten equations define saturation when the fluid pressure is atmospheric (that is, $H_p = 0$). These equations are

$$\theta = \begin{cases} \theta_\mathrm{r} + \mathrm{Se}(\theta_\mathrm{s} - \theta_\mathrm{r}) & H_p < 0 \\ \theta_\mathrm{s} & H_p \geq 0 \end{cases}$$

$$\mathrm{Se} = \begin{cases} \dfrac{1}{[1 + |\alpha H_p|^n]^m} & H_p < 0 \\ 1 & H_p \geq 0 \end{cases}$$

$$C = \begin{cases} \dfrac{\alpha m}{1-m}(\theta_\mathrm{s} - \theta_\mathrm{r})\mathrm{Se}^{\frac{1}{m}}\left(1 - \mathrm{Se}^{\frac{1}{m}}\right)^m & H_p < 0 \\ 0 & H_p \geq 0 \end{cases}$$

$$k_\mathrm{r} = \begin{cases} \mathrm{Se}^l\left[1 - \left(1 - \mathrm{Se}^{\frac{1}{m}}\right)^m\right]^2 & H_p < 0 \\ 1 & H_p \geq 0 \end{cases}$$

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

$$\theta = \begin{cases} \theta_r + \mathrm{Se}(\theta_s - \theta_r) & H_p < -\frac{1}{\alpha} \\ \theta_s & -\frac{1}{\alpha} \le H_p \end{cases}$$

$$\mathrm{Se} = \begin{cases} \frac{1}{|\alpha H_p|^n} & H_p < -\frac{1}{\alpha} \\ 1 & -\frac{1}{\alpha} \le H_p \end{cases}$$

$$C = \begin{cases} \frac{-n}{H_p}(\theta_s - \theta_r)\frac{1}{|\alpha H_p|^n} & H_p < -\frac{1}{\alpha} \\ 0 & -\frac{1}{\alpha} \le H_p \end{cases}$$

$$k_r = \begin{cases} \mathrm{Se}^{\frac{2}{n} + l + 2} & H_p < -\frac{1}{\alpha} \\ 1 & -\frac{1}{\alpha} \le H_p \end{cases}$$

COMSOL Multiphysics also provides user-defined options for those who want to incorporate experimental data or arbitrary expressions to define these relationships. COMSOL Multiphysics supplies options to enter the data through tables or files, methods to interpolate between data points, and numerical differentiation.

Boundary Conditions

The predefined boundary conditions supplied by the Richards' Equation application mode appear similar to those provided with the Darcy's law application mode. For details about the physical meaning behind this mix of Dirichlet, Neumann, and Cauchy conditions, please refer to the discussion on pressure analysis with the Darcy's law application modes. The boundary conditions are:

$p = p_0$ Pressure

$p = 0$ Atmosphere or gauge

$\mathbf{n} \cdot \frac{\kappa}{\eta} k_r(\nabla p + \rho_f g \nabla D) = 0$ Zero flux/Symmety

$\mathbf{n} \cdot \frac{\kappa}{\eta} k_r(\nabla p + \rho_f g \nabla D) = N_0$ Inward flux

$\mathbf{n} \cdot \frac{\kappa}{\eta} k_r(\nabla p + \rho_f g \nabla D) = N_0 + R_b[p_b - p + D_b - D]$ Mixed

In these equations, $\mathbf{n}$ represents the normal to the boundary, p_0 is the specified pressure, N_0 a specified flux, R_b conductance to flow in a thin layer adjacent to the boundary, and p_b the pressure at the edge of the resistive layer. 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 the gravitational potential, as defined on D.

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The Brinkman Equations

Introduction

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 equation. Consequently, this application mode 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.

The dependent variables in the Brinkman equations are the directional velocities and pressure. The flow field balances momentum in the x, y, and z directions and preserves continuity with

$$\frac{\rho}{\varepsilon_{\mathrm{p}}}\frac{\partial \mathbf{u}}{\partial t}+\left(\frac{\eta}{\kappa}+Q\right)\mathbf{u} = \nabla\cdot\left[p\mathbf{I}+\frac{1}{\varepsilon_{\mathrm{p}}}\left\{\eta(\nabla\mathbf{u}+\nabla\mathbf{u}^T)-\left(\frac{2\eta}{3}-\kappa_{\mathrm{dv}}\right)(\nabla\cdot\mathbf{u})\mathbf{I}\right\}\right]+\mathbf{F}$$

$$\rho\nabla\cdot\mathbf{u} = Q$$

where ρ denotes the density, η the viscosity, k the permeability, ε_{p} the porosity, $\mathbf{u}$ the velocity, p the pressure, κ_{dv} the dilatational viscosity, and $\mathbf{F}$ a force term. Q is an optional mass source term that can be useful for modeling condensation in porous media. Some scientists argue that the permeability for the Brinkman equations and Darcy's law differ. You can enter arbitrary force terms, $\mathbf{F}$, to model directed forces including gravity and small compressibility effects. For example, see the example of density-driven flow driven by temperature changes "Free Convection in Porous Media" on page 340 of the *Earth Science Module Model Library.*

Subdomain Equations and Stabilization

The Brinkman Equations application mode is fully integrated with the Incompressible Navier-Stokes application mode. You can switch between free flow and porous media flow in a given subdomain by selecting the **Flow in porous media (Brinkman equations)** check box in the **Subdomain Settings** dialog box. Otherwise, the settings on the Physics page are the same as for the Incompressible Navier-Stokes application mode.

Numeric stabilization is not available when you use the Brinkman Equations application mode, because the Brinkman equations lack the convective term that makes it important to stabilize the Navier-Stokes

Boundary Conditions

The Brinkman Equations application mode supports the same boundary conditions as the Incompressible Navier-Stokes application mode. See “Boundary Conditions” on page 31 for information about these boundary conditions.

Solution Strategy—Initial Conditions

Solving the Brinkman equations and the Navier-Stokes equations often requires a reasonable initial guess for directional velocities and pressure, even for steady-state flow systems. Simple expressions are often sufficient. For vertical upward flow, for instance, you might set v equal to some positive value and u to a very small number ε.

Occasionally you need a relatively refined snapshot of pressure and velocity for an initial guess. A reasonable strategy is to solve a similar model and use the results from the dummy simulation as the initial guess. In COMSOL Multiphysics it is straightforward to reach a good initial condition using the parametric solver. Here the dummy simulation solves directly on your model except that it varies a parameter, typically viscosity η, velocity $\mathbf{u}$, or density ρ. The parametric solver increases or decreases the parameter value in a series of simulations until the problem solves for the true parameter value. In modeling gas flow, for instance, the solver moves incrementally from a high viscosity to the true value.

The Incompressible Navier-Stokes Equations

The 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 application mode couples arbitrarily with other physics 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 application mode is useful for flows of Newtonian fluids where the density can be assumed to be constant or nearly constant.

In theory, these equations describe laminar as well as turbulent flows. In practice however, the mesh resolution required to simulate turbulence with this application mode makes such an approach impractical.

Subdomain Equations

The Incompressible Navier-Stokes application mode assumes that the fluid is incompressible; that is, that ρ is constant or nearly constant. This is the case for all fluids under normal conditions and also for gases at low velocities. For constant ρ, the continuity equations is

$$\nabla \cdot \mathbf{u} = 0 \qquad (3\text{-}5)$$

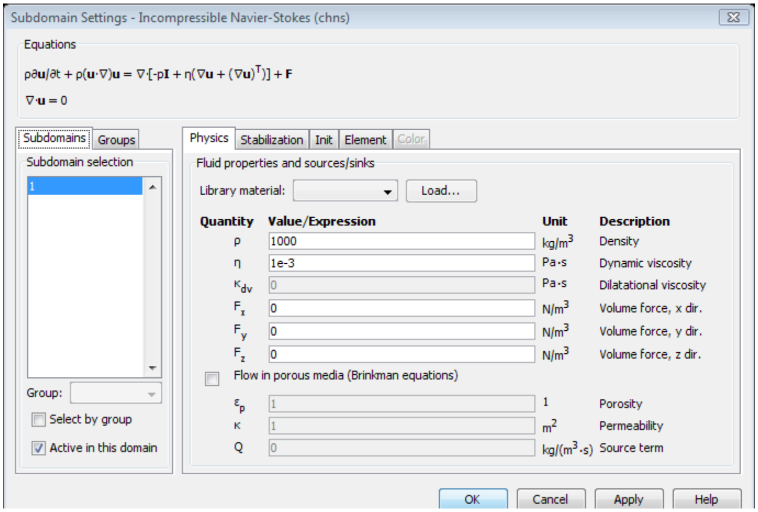
and the stress tensor τ becomes

$$\tau = \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

These assumptions put together give the following momentum equations:

$$\rho\frac{\partial\mathbf{u}}{\partial t} + (\rho\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nabla\cdot(\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) + \mathbf{F} \qquad (3\text{-}6)$$

The equations used by the application mode are displayed in the **Subdomain Settings** dialog box. Here, you also specify the physical properties of the fluid (see Figure 3-3).



$\rho\partial\mathbf{u}/\partial t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$

$\nabla\cdot\mathbf{u} = 0$

Quantity	Value/Expression	Unit	Description
ρ	1000	kg/m^3	Density
η	1e-3	Pa·s	Dynamic viscosity
κ_{dv}	0	Pa·s	Dilatational viscosity
F_x	0	N/m^3	Volume force, x dir.
F_y	0	N/m^3	Volume force, y dir.
F_z	0	N/m^3	Volume force, z dir.

☐ Flow in porous media (Brinkman equations)

Quantity	Value/Expression	Unit	Description
ε_p	1	1	Porosity
κ	1	m^2	Permeability
Q	0	kg/(m^3·s)	Source term

Figure 3-3: The Subdomain Settings dialog box for 3D incompressible Navier-Stokes equations.

Reynolds Number

Scientists often use the dimensionless Reynolds number, Re, to characterize the flow regime. It denotes the ratio of inertial to viscous forces as in

$$\mathrm{Re} = \frac{du_0\rho}{\eta}$$

where d is a characteristic length. As Re increases, flow moves from laminar to turbulent.

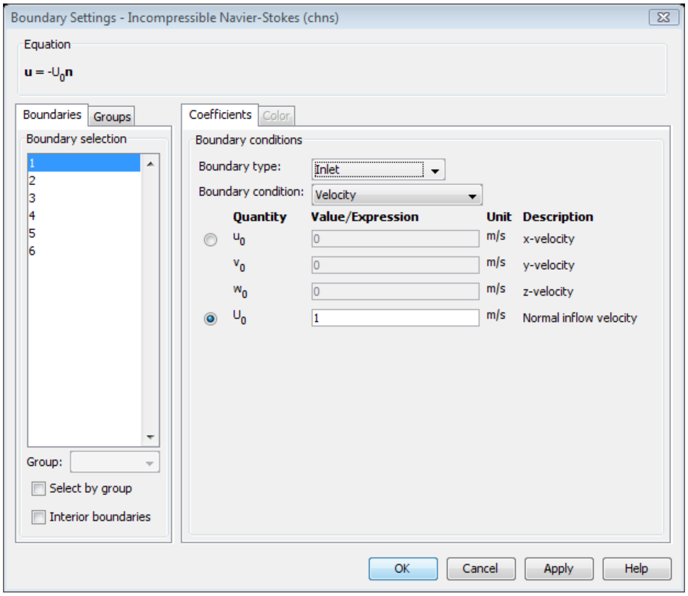
The Navier-Stokes application mode automatically calculates the cell Reynolds number using the element length h for d and the magnitude of the velocity vector U for u_0. Modeling turbulent flow with the Navier-Stokes equations requires a large number of nodes to resolve small eddies that can move through the flow in seemingly random patterns in space and time. These types of simulations demand a large computational effort that outstrips the capacity of most computers. Keeping track of Re is helpful for modeling fast flows.

Boundary Conditions

The boundary conditions for the Incompressible Navier-Stokes application mode are grouped into the following types:

- Wall
  - No slip (default)
  - Slip
  - Sliding wall
  - Moving/leaking wall
- Inlet
  - Velocity (default)
  - Pressure, no viscous stress
  - Laminar inflow
- Outlet
  - Velocity
  - Pressure
  - Pressure, no viscous stress (default)
  - No viscous stress
  - Normal stress
  - Laminar outflow
- Symmetry boundary
  - Symmetry (default)
  - Axial symmetry (2D axisymmetry only)
- Open boundary
  - Normal stress (default)
  - No viscous stress
- Stress
  - General stress (default)
  - Normal stress
  - Normal stress, normal flow

You specify a boundary condition in the **Boundary Settings** dialog box, where you first select the appropriate **Boundary type** and then a **Boundary condition**.



Equation

$\mathbf{u} = -U_0\mathbf{n}$

Boundary type: Inlet

Boundary condition: Velocity

	Quantity	Value/Expression	Unit	Description
○	u_0	0	m/s	x-velocity
	v_0	0	m/s	y-velocity
	w_0	0	m/s	z-velocity
●	U_0	1	m/s	Normal inflow velocity

Figure 3-4: Boundary Settings dialog box for the Incompressible Navier-Stokes application mode.

If a mathematical formulation describes more than one type of physical boundary condition, it can appear in more than one boundary type. However, every possible use of a single mathematical formulation cannot be covered. Hence, the boundary types should be regarded as guidelines, not as restrictions on the applicability of the formulations.

The theory of most boundary conditions can be found in Ref. 1.

WALL

These boundary conditions describe the existence of a solid wall.

No Slip

This is the standard and default boundary condition for a stationary solid wall. The condition prescribes

$$\mathbf{u} = \mathbf{0}$$

that is, that the fluid at the wall is not moving.

Moving/Perforated Wall

If the wall moves, so must the fluid. Hence, this boundary condition prescribes

$$\mathbf{u} = \mathbf{u}_{\mathrm{w}}$$

Note that setting this boundary condition does not automatically cause the associated wall to move. The section "The Moving Mesh Application Mode" on page 455 of the *COMSOL Multiphysics Modeling Guide* describes how to set up a model with moving boundaries.

You can also use the Moving/perforated wall boundary condition to simulate a wall where fluid is leaking into or leaving through a perforated wall.

Sliding Wall

If you use this boundary condition, the wall is assumed to behave like a conveyor belt, that is, that the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

In two space dimensions (2D), the tangential direction is unambiguously defined by the direction of the boundary. However, the situation becomes more complicated in 3D. For this reason, this boundary condition has slightly different definitions in the different space dimensions.

2D and Axial Symmetry The velocity is given as a scalar U_{w} and the condition prescribes

$$\mathbf{u} \cdot \mathbf{n} = 0$$
$$\mathbf{u} \cdot \mathbf{t} = \mathrm{U}_{\mathrm{w}}$$

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

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

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

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 may be 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:

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

where **t** is a tangential vector to the boundary.

INLET

This boundary type contains different ways to specify conditions on a boundary where the fluid is supposed to enter the domain. Notice that the formulations contained in this boundary type all appear, some of them slightly modified, in the Outflow boundary type as well. Hence, there is nothing in the mathematical formulations that prevents a fluid from leaving the domain through boundaries where you have specified the Inlet boundary type.

Velocity

This boundary condition offers two ways to specify an inlet velocity. The first is to set the velocity equal to a given vector $\mathbf{u}_0$:

$$\mathbf{u} = \mathbf{u}_0$$

The other is to specify a normal inflow velocity:

$$\mathbf{u} = -\mathbf{n}\mathrm{U}_0$$

Note that the boundary normal, $\mathbf{n}$, points out of the domain.

Pressure, No Viscous Stress

This boundary condition specifies vanishing viscous stress along with a Dirichlet condition on the pressure:

$$\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} = \mathbf{0}, \qquad p = p_0$$

It is a numerically stable boundary condition that admits total control of the pressure level along the entire boundary. However, if the inflow is not normal to the boundary, this condition is an overspecification. In the case that your solution turns out to have a non-normal inflow velocity, there are two choices. Either, move the boundary farther away to a location where the inflow is normal to the boundary or, use a stress type boundary condition described on page 37.

Note that this condition is identical to the Pressure, no viscous stress condition for Outflow boundaries. Hence, depending on the pressure field in the rest of the subdomain, a boundary with this condition can very well become an outflow boundary.

OUTFLOW

This boundary type contains different ways to specify conditions on a boundary where the fluid exits the domain. Note that all of the formulations in this type can be found, possibly slightly modified, in other boundary types as well. Hence, there is nothing in the mathematical formulations that prevent a fluid from entering the domain through boundaries where you have set the Outflow boundary type.

Setting outlet conditions for the Navier-Stokes equations is not a trivial task. A general rule of thumb, however, is that if there is something interesting happening at an outflow boundary, extend the computational domain to include this phenomenon.

Velocity

This boundary condition offers two ways to specify an outlet velocity. The first is to set the velocity equal to a given vector $\mathbf{u}_0$:

$$\mathbf{u} = \mathbf{u}_0$$

The other is to specify a normal outlet velocity:

$$\mathbf{u} = \mathbf{n}\mathrm{U}_0$$

Observe that the boundary normal, $\mathbf{n}$, is pointing out of the domain.

Pressure, No Viscous Stress

This boundary condition specifies vanishing viscous stress along with a Dirichlet condition on the pressure:

$$\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} = \mathbf{0}, \qquad p = p_0$$

It is a numerically stable boundary condition that admits total control of the pressure level at the whole boundary. However, if the outflow is not normal to the boundary, this condition is an overspecification. In the case that your solution turns out to have a non-normal outflow velocity, there are two choices. Either move the boundary farther away to a location where the outflow is normal to the boundary or use a stress type boundary condition described on page 37.

Note that this condition is identical to the Pressure, no viscous stress condition for Inflow boundaries. Hence, depending on the pressure field in the rest of the subdomain, a boundary with this condition can very well become an inflow boundary.

Pressure

This boundary condition prescribes only a Dirichlet condition for the pressure:

$$p = p_0$$

Use this boundary condition only for high Reynolds number outflow boundaries; that is, boundaries where the cell Reynolds number $\mathrm{Re}^c = \rho|\mathbf{u}|h/(2\eta) >> 1$ (h is the local mesh element size). It is far less stable than the Pressure, no viscous stress boundary condition, but it is consistent with a non-normal outflow velocity. The cell Reynolds number is available for postprocessing using the default name `cellRe_ns`.

No Viscous Stress

Prescribes vanishing viscous stress:

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

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. It should however be combined with a point constraint on the pressure to be numerically stable (see “Point Settings” on page 38).

Normal Stress

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

$$(-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -\mathrm{f}_0\mathbf{n}$$

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

$$p = 2\eta\frac{\partial u_n}{\partial n} + \mathrm{f}_0 \qquad (3\text{-}7)$$

If $\partial u_n/\partial n$ is small, Equation 3-7 can be interpreted as $p \approx \mathrm{f}_0$.

SYMMETRY BOUNDARY

Prescribes no penetration and vanishing shear stresses:

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

In 2D Axial Symmetry, the above formulation is called **Symmetry**.

Axial Symmetry

This boundary condition is only available in 2D Axial Symmetry. Use it on all boundaries with coordinate $r = 0$. It prescribes $u_r = 0$ and vanishing stresses in the z direction.

OPEN BOUNDARY

You can use this boundary type on boundaries that are open to large volumes of fluid. Fluid can both enter and leave the domain on boundaries with this type of condition.

No Viscous Stress

Prescribes vanishing viscous stress:

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

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. It should however be combined with a point constraint on the pressure to be numerically stable (see "Point Settings" on page 38).

Normal Stress

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

$$(-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -\mathrm{f}_0\mathbf{n}$$

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

$$p = 2\eta\frac{\partial u_n}{\partial n} + \mathrm{f}_0 \qquad (3\text{-}8)$$

If $\partial u_n/\partial n$ is small, Equation 3-8 can be interpreted as $p \approx \mathrm{f}_0$.

STRESS

This type of boundary condition represents a very general class of conditions also known as traction boundary conditions.

General Stress

The total stress on the boundary is set equal to a given stress $\mathbf{F}$:

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

This boundary condition implicitly sets a constraint on the pressure that for 2D flows can be written

$$p = 2\eta\frac{\partial u_n}{\partial n} - \mathbf{n}\cdot\mathbf{F} \tag{3-9}$$

If $\partial u_n/\partial n$ is small, Equation 3-9 can be interpreted as $p \approx -\mathbf{n}\cdot\mathbf{F}$.

Normal Stress

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

$$(-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = -\mathrm{f}_0\mathbf{n}$$

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

$$p = 2\eta\frac{\partial u_n}{\partial n} + \mathrm{f}_0 \tag{3-10}$$

If $\partial u_n/\partial n$ is small, Equation 3-10 can be interpreted as $p \approx \mathrm{f}_0$.

Normal Stress, Normal Flow

In addition to the stress condition set in the Normal stress condition, this condition also prescribes that there must be no tangential velocities on the boundary:

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

Also this boundary condition implicitly sets a constraint on the pressure that for 2D flows can be written

$$p = 2\eta\frac{\partial u_n}{\partial n} + \mathrm{f}_0 \tag{3-11}$$

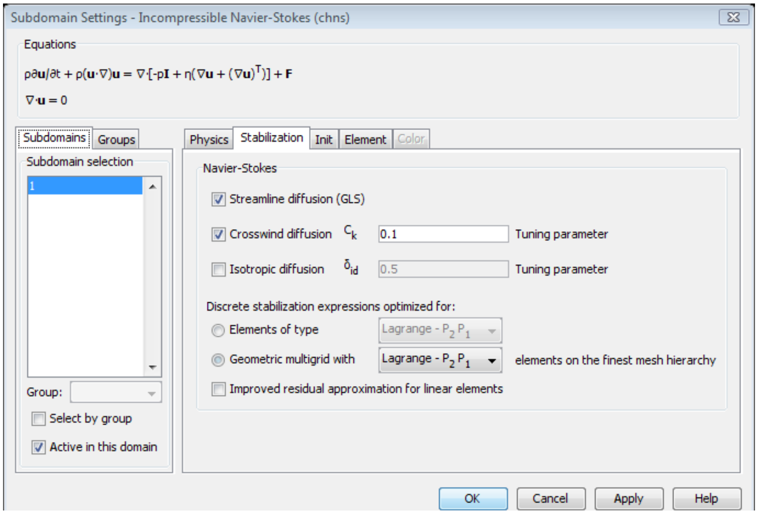
If $\partial u_n/\partial n$ is small, Equation 3-11 can be interpreted as $p \approx \mathrm{f}_0$.

Point Settings

If it is not possible to specify the pressure level using a boundary condition, the pressure must be set in some other way, for example, by specifying a fixed pressure at a point. You find a dialog box for **Point Settings** on the **Physics** menu.

Numerical Stability—Stabilization Techniques

The momentum equations (see Equation 3-6) are (nonlinear) convection-diffusion equations. As described in Chapter 17, “Stabilization Techniques,” of the *COMSOL Multiphysics Modeling Guide* such equations are unstable if discretized using the Galerkin finite element method. Stabilized finite element methods are therefore necessary in order to obtain physical solutions. You control the stabilization settings from the **Stabilization** page in the **Subdomain Settings,** which appears in Figure 3-5.



Subdomain Settings - Incompressible Navier-Stokes (chns)

Equations

$\rho\partial\mathbf{u}/\partial t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$

$\nabla\cdot\mathbf{u} = 0$

Subdomain selection: 1

Group:

☐ Select by group

☑ Active in this domain

Navier-Stokes

☑ Streamline diffusion (GLS)

☑ Crosswind diffusion c_k 0.1 Tuning parameter

☐ Isotropic diffusion δ_{id} 0.5 Tuning parameter

Discrete stabilization expressions optimized for:

○ Elements of type Lagrange - P_2 P_1

● Geometric multigrid with Lagrange - P_2 P_1 elements on the finest mesh hierarchy

☐ Improved residual approximation for linear elements

Figure 3-5: The Stabilization page of the Subdomain Settings dialog box.

There are three types of stabilization available in the Incompressible Navier-Stokes application mode:

- Streamline diffusion (GLS)
- Crosswind diffusion
- Isotropic diffusion

For optimal functionality, the exact weak formulations and constants of GLS and crosswind diffusion depend on the order of the basis functions (elements). To control this, there are two option buttons, each with its corresponding list, at the bottom of the **Stabilization** page shown in Figure 3-5. In most cases, the model utilizes only one element type. If this is the case, select this type from the **Elements of type** list. This is the default setting for all dimensions but 3D.

However, when using the geometric multigrid (GMG) solver/preconditioner, the equations can be discretized with different elements on the different multigrid hierarchies. Then select from the element type that is used on the finest mesh hierarchy from the **Geometric multigrid with** list. This is the default setting for 3D because the default solver for in 3D is BiCGStab with geometric multigrid as the preconditioner. The resulting weak expressions then take forms adapted to multigrid hierarchies created in a way equivalent to the hierarchy generation method that you get when you choose **Lower element order first (any)** from the **Hierarchy generation method** list in the **Linear System Solver Settings** dialog box (see "Constructing a Multigrid Hierarchy" on page 560 of the *COMSOL Multiphysics Reference Guide*).

The values of constants of the GLS and crosswind diffusion follow Ref. 2 and Ref. 3 and cannot be changed without performance losses.

Streamline diffusion and crosswind diffusion are functional only for the element types available in the lists on the **Stabilization** page.

STREAMLINE DIFFUSION (GLS)

For strongly coupled system of equations, the streamline diffusion must be applied to the whole system of equations, not only to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 4) and were later extended to Galerkin least-squares (GLS) applied to the Navier-Stokes equations (Ref. 5) which is the form that COMSOL supports. The time scale tensor is the diagonal tensor presented in Ref. 6.

Streamline diffusion is active per default since it is necessary when the flow is dominated by convection.

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

CROSSWIND DIFFUSION

Crosswind diffusion can also be formulated for system of equations and when applied to the Navier-Stokes equations it becomes a chock capturing operator. COMSOL supports the formulation in Ref. 5 with shock capturing viscosity taken from Ref. 7.

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

The tuning parameter, C_k, controls the amount of crosswind diffusion introduced in the model. The recommended range for low Mach number flows and incompressible flows is $0 < C_k < 0.5$ (C_k=0 means no diffusion at all). The value must not be neither space, nor time dependent.

Crosswind diffusion is active per default since it makes it easier to obtain a solution even if the mesh is not perfect. It is, however, advisable to investigate the influence C_k.

Crosswind diffusion also has the effect that iterative solvers can use inexpensive presmoothers such as SSOR (see "Solver Settings" on page 44). If you deactivate crosswind diffusion, you must change all applications of SSOR to Vanka (see "Preconditioners for the Iterative Solvers" on page 555 in the *COMSOL Multiphysics Reference Guide*).

ISOTROPIC DIFFUSION

Isotropic diffusion adds diffusion to the momentum equations of the Navier-Stokes equations in the same way as described in "Isotropic Diffusion" on page 486 of the *COMSOL Multiphysics Modeling Guide*. The continuity equation gain no extra stability.

IMPROVED RESIDUAL APPROXIMATION FOR LINEAR ELEMENTS

Both GLS and crosswind diffusion evaluate the residuals of the Navier-Stokes equations to determine the amount of diffusion. The residuals of the momentum equations contain second order derivatives of the velocity which, if linear elements are used, are evaluated to zero. The impact of this is small if the flow is dominated by convection where

$$\partial\mathbf{u}/\partial t + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p \tag{3-12}$$

is a good approximation of the momentum equations. Equation 3-12 is not a good approximation for flows dominated by viscous effects, however, and if the mesh is coarse, the result can be that the pressure field contains small oscillations.

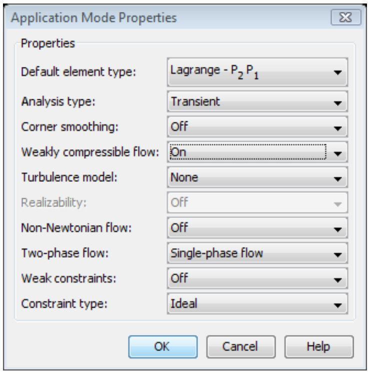
The oscillations can be removed by refining the mesh. An alternative is to select the **Improved Residual Approximation for Linear Elements** check box shown in Figure 3-5. The viscous terms are then reconstructed by polynomial-preserving recovery (see "Using Special Operators" on page 163 of the *COMSOL Multiphysics User's Guide*).

The polynomial-preserving recovery makes the equation system more complicated and thereby more expensive to solve.

The improved residuals can be useful if the Navier-Stokes equations are part of a multiphysics problem and you cannot afford to refine the mesh.

Corner Smoothing

You find the **Corner smoothing** property in the **Application Mode Properties** dialog box. It can be a useful property when the model contains walls with slip conditions, as described below.


Application Mode Properties

Properties

Default element type: Lagrange - P_2 P_1

Analysis type: Transient

Corner smoothing: Off

Weakly compressible flow: On

Turbulence model: None

Realizability: Off

Non-Newtonian flow: Off

Two-phase flow: Single-phase flow

Weak constraints: Off

Constraint type: Ideal

Figure 3-6: The Application Mode Properties dialog box where Corner smoothing can be turned on and off.

Consider the situation sketched in Figure 3-7. At the point where the boundaries Γ_1 and Γ_2 intersect, there are two boundary normals, one for Γ_1 and one for Γ_2. These two normals are denoted $\mathbf{n}_{\Gamma 1}$ and $\mathbf{n}_{\Gamma 2}$ in Figure 3-7. If the boundaries now both have no-penetration condition, there are two Dirichlet conditions at the point of intersection, namely

$$\mathbf{n}_{\Gamma 1} \cdot \mathbf{u} = 0 \qquad (3\text{-}13)$$

and

$$\mathbf{n}_{\Gamma 2} \cdot \mathbf{u} = 0 \qquad (3\text{-}14)$$

The only way that both Equation 3-13 and Equation 3-14 can be fulfilled is if $\mathbf{u} \equiv \mathbf{0}$ at the point of intersection. This is not always the expected solution, however.

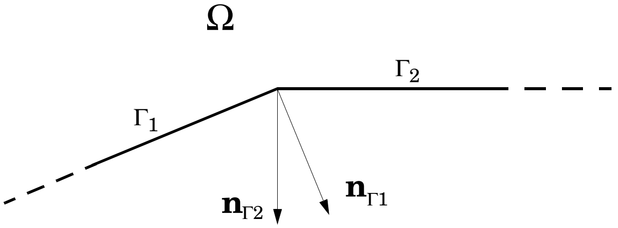


Figure 3-7: Intersection between the boundaries Γ_1 *and* Γ_2*.* $\mathbf{n}_{\Gamma 1}$ *and* $\mathbf{n}_{\Gamma 2}$ *are the boundary normals prescribed by* Γ_1 *and* Γ_2 *respectively.* Ω *is the computational domain.*

When corner smoothing is activated, any Dirichlet condition $d(\mathbf{n}) = 0$ is replaced by $d(\mathbf{n}_\mathrm{w}) = 0$, where $\mathbf{n}_\mathrm{w}$ is a vector of dependent boundary variables whose solution in each point is the average of all normals in that point. In the current example, equations 3-13 and 3-14 are replaced with

$$\mathbf{n}_\mathrm{w} \cdot \mathbf{u} = \mathbf{0} \qquad (3\text{-}15)$$

and $\mathbf{n}_\mathrm{w}$ has the solution $\mathbf{n}_\mathrm{w} = (\mathbf{n}_{\Gamma 1} + \mathbf{n}_{\Gamma 2})/2$. Equation 3-15 can then be satisfied for $\mathbf{u} \neq \mathbf{0}$.

Application Mode Variables

A number of variables and physical quantities are available for postprocessing and for use in equations and boundary conditions. They appear in the following table (where x_i denotes the various space coordinate directions and, in the **Type** column, V represents vertices (points, B represents boundaries, and S represents subdomains):

NAME	TYPE	DESCRIPTION	EXPRESSION
u, v, (w)	B S V	x_i velocity	u, v, w
p	B S	Pressure	p
U	B S	Velocity field	$\sqrt{\sum_i (u_i)^2}$
V	S	Vorticity	$\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$ (2D)

NAME	TYPE	DESCRIPTION	EXPRESSION
`Vxi`	S	Vorticity	x_i components of $\nabla \times \mathbf{u}$ (3D)
`rho`	S	Density	ρ
`eta`	S	Dynamic viscosity	η
`F_xi`	S	Volume force, x_i dir.	x_i components of $\mathbf{F}$
`K_xi`	B	Viscous force per area, x_i component	$\sum_j n_j \eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$
`T_xi`	B	Total force per area, x_i component	$\sum_j n_j\left[-p\delta_{ij} + \eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]$
`cellRe`	S	Cell Reynolds number	$\frac{\rho\lvert\mathbf{u}\rvert h}{\eta}$
`res_ui_c`	S	Equation residual, u_i component	$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \mathbf{F}$ $-\nabla \cdot [\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)]$ (u_i component)
`res_sc_ui_c`	S	Shock capturing residual, u_i component	$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \mathbf{F}$ (u_i component)
`beta_xi`	S	Convective field, x_i component	ρu_i
`Dm`	S	Mean diffusion coefficient	η
`da`	S	Total time-scale factor	ρ

Note: To form the complete application mode variable names, add a suffix consisting of an underscore and the application mode name (default: `ns`), for example, `V_ns`. (This does not apply to the dependent variables for the velocities and pressure.)

Solver Settings

LINEAR SYSTEM SOLVER

The recommended solver type for small and medium-sized fluid-flow problems is a direct solver, and the PARDISO direct solver is the default solver for 1D and 2D models. It is not as robust as UMFPACK or SPOOLES but is more memory efficient.

3D problems are often too large to solve using a direct solver. The default solver is BiCGStab with the geometric multigrid (GMG) preconditioner. The GMG preconditioner uses the SSOR preconditioner/smoother as the presmoother and postsmoother. It is possible to use SSOR thanks to the GLS streamline diffusion and to the crosswind diffusion (see "Numerical Stability—Stabilization Techniques" on page 39). If you deactivate any of these stabilization settings, then you must replace the SSOR smoothers by the Vanka preconditioner/smoother (see "The Vanka Algorithm" on page 570 in the *COMSOL Multiphysics Reference Guide*.).

For more information about the solvers, see Chapter 6, "Solving the Model," on page 377 in the *COMSOL Multiphysics User's Guide*.

TRANSIENT SOLVER SETTINGS

The transient Incompressible Navier-Stokes application mode uses per default the generalized-α time-stepping method (see "The Time-Dependent Solver" on page 391 of the *COMSOL Multiphysics User's Guide*) with manual time step control.

The time step for the transient Incompressible Navier-Stokes application mode is calculated from the CFL number:

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

The Navier-Stokes application mode contains a variable `dt_cfl_gn_app` that corresponds to a CFL number equal to one. *n* is the index of the geometry on which the application mode is active and *app* is the application mode name. As an example, assume that the application mode name is ns and that the application mode is active on geometry 2. The time step variable is then `dt_cfl_g2_ns`.

`dt_cfl_gn_app` is defined by

$$\texttt{dt\_cfl\_g}\mathit{n}\texttt{\_}\mathit{app} = \min_{\Omega_e}\left(\frac{h}{\max(|\mathbf{u}|, \mathrm{f_{vv}}\mathrm{u_{diff}})}\right)$$

where Ω_e is the set of all mesh cells in geometry *n* on subdomains where the Navier-Stokes is active. $\mathrm{u_{diff}}$ is a diffusive velocity scale equal to $\eta/(\rho h)$. The argument $\mathrm{f_{vv}}\mathrm{u_{diff}}$ is necessary to prevent the time step from becoming too large when $|\mathbf{u}|$ is small. Because $\mathrm{u_{diff}}$ is often extremely small, the algorithm multiplies it by a factor, $\mathrm{f_{vv}}$, which per default is 10.

A necessary condition for explicit time stepping techniques to be stable is that the CFL number is smaller than one. COMSOL uses implicit schemes which are stable for any

Δt. Large Δt has the advantage that the computation can be completed in few time steps. There are however two drawbacks:

- The solver introduces numerical diffusion that increases with Δt. In other words, using large Δt means that the result becomes less accurate compared to using small Δt.
- The equation system becomes harder to solve for large Δt. That is, more computational work is required to complete each time step.

A compromise between efficiency and accuracy is to use a Δt such that $2 \le \mathrm{CFL} \le 10$. The default is $\Delta t = 5 \cdot$`dt_cfl_`*app*, and you find this setting on the **Time Stepping** page in the **Solver Parameters** dialog box.

You can increase the time step if the model contains only very slow transients. Conversely, if the solver repeatedly fails to solve the nonlinear system (see "The Time-Dependent Solver Log" on page 452 of the *COMSOL Multiphysics User's Guide*), then decrease the time step.

In situations where the viscosity is high or if the model has a very dense mesh, f_{vv}=10 can result in very small time steps. The factor f_{vv}, the viscous velocity factor, is available as an application scalar variable named `visc_vel_fact_`*app*, and you can set it to any suitable value in the **Application Scalar Variables** dialog box (choose **Scalar Variables** from the **Physics** menu).

In some models the transient behavior is not guided by the Navier-Stokes equations, and the CFL condition can be overly restrictive. If this is the case, go to the **Time Stepping** page in the **Solver Parameters** dialog box. Then change the **Time steps take by solver** to **Free** or edit the **Time step** expression to take the time scale of the guiding physics into account.

ADVANCED SOLVER SETTINGS

For a flow that is parallel to a coordinate axis, the automatic scaling feature in COMSOL Multiphysics does not work if you use the nonlinear stationary solver. For such cases, turn off the scaling feature or use manual scaling; see "Scaling of Variables and Equations" on page 531 of the *COMSOL Multiphysics Reference Guide*. The problem occurs when one solution component is on average zero.

Khan and Richardson Force for Particle Tracing

The *Khan and Richardson force* is available for particle tracing plots in the Incompressible Navier-Stokes application mode and other application modes for fluid dynamics in the COMSOL Multiphysics products.

BACKGROUND

The force expression that the software uses is derived partly using experimental results, and it is valid for a wide range of Reynolds numbers, stretching from creeping flow toward the turbulent regime (Ref. 8).

The following equation describes the total force that a fluid exerts on an immersed spherical particle:

$$F = \pi r_p^2\rho(\bar{u}-\bar{u}_p)^2(1.84(\mathrm{Re}_p)^{-0.31}+0.293(\mathrm{Re}_p)^{0.06})^{3.45}$$

where the definition of the particle Reynolds number, Re_p, is

$$\mathrm{Re}_p = (|\bar{u}-\bar{u}_p|2r_p\rho)/\eta\ .$$

The orientation of a given force component (for example, positive or negative x-component) is determined by the sign of the corresponding component in the vector difference $\bar{u}-\bar{u}_p$, because this determines whether the fluid is accelerating or slowing down the particle in that direction.

USING THE KHAN AND RICHARDSON FORCE FOR PARTICLE TRACING

The Khan and Richardson force is the default selection in the **Predefined forces** list on the **Particle Tracing** tab.

There is one parameter in this force expression: the particle radius r_p, which you define by clicking the **Parameters** button. Table 3-1 shows the default values for this parameter:

TABLE 3-1: PARAMETER FOR THE KHAN AND RICHARDSON FORCE

PARAMETER NAME IN EQUATION	DESCRIPTION	DEFAULT VALUE	DEFAULT VARIABLE NAME
r_p	particle radius	10^{-4} m	`partr`

The particle mass appears in the force equation, and you enter its value in the **Mass** edit field. The default value for the particle mass is $m_p = (4\pi/3)\cdot 10^{-9}$ kg, which is the mass of a particle with the same density as water and a radius of 10^{-4} m, which is the default radius.

Note: The default settings work for models that use SI units.

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Flow with Variable Density

The Weakly Compressible Navier-Stokes application mode is an extension of the Incompressible Navier-Stokes application mode for fluid flow where the density is not constant (weakly compressible flow).

Weakly Compressible Navier-Stokes

This application mode contains the fully compressible formulation of the continuity equation and momentum equations:

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \\ &\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left(\eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \left(\frac{2}{3}\eta - \kappa_{\mathrm{dv}} \right) (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F} \end{aligned} \qquad (3\text{-}16)$$

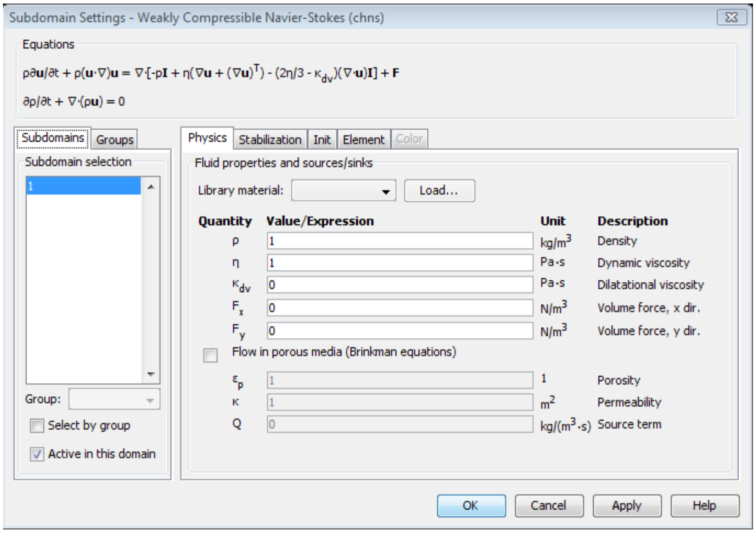
where

- ρ is the density (kg/m^3)
- $\mathbf{u}$ is the velocity vector (m/s)
- p is pressure (Pa)
- η is the dynamic viscosity (Pa·s)
- κ_{dv} is the dilatational viscosity (Pa·s)
- $\mathbf{F}$ is the body force vector (N/m^3)

The stress tensor used in Equation 3-16 describes a Newtonian fluid but with an extra term κ_{dv}. This term expresses the deviation from Stokes' assumption, which states that the fluid particles are in thermodynamic equilibrium with their neighbors. It is very rare that a fluid shows a significant deviation from Stokes' assumption, and κ_{dv} is therefore by default set to zero.

SUBDOMAIN SETTINGS

The **Subdomain Settings** dialog box is shown in Figure 3-8. The set of properties on the **Physics** page for the Weakly Compressible Navier-Stokes application mode is the same as the one for the Incompressible Navier-Stokes application mode, with the addition of the dilatational viscosity, κ_{dv}.



$\rho\partial\mathbf{u}/\partial t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - (2\eta/3 - \kappa_{dv})(\nabla\cdot\mathbf{u})\mathbf{I}] + \mathbf{F}$

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

Quantity	Value/Expression	Unit	Description
ρ	1	kg/m^3	Density
η	1	Pa·s	Dynamic viscosity
κ_{dv}	0	Pa·s	Dilatational viscosity
F_x	0	N/m^3	Volume force, x dir.
F_y	0	N/m^3	Volume force, y dir.

☐ Flow in porous media (Brinkman equations)

ϵ_p	1	1	Porosity
κ	1	m^2	Permeability
Q	0	kg/(m^3·s)	Source term

Figure 3-8: The Subdomain Settings dialog box for the Weakly Compressible Navier-Stokes application mode. Physics page.

Typically, the Weakly Compressible Navier-Stokes application mode is coupled to a heat equation that describes the variations in the temperature field for nonisothermal flow. The stabilization settings on the **Stabilization** page (see "Numerical Stability—Stabilization Techniques" on page 39) reflect this by adding two option buttons, **Isothermal flow** (the default) and **Non-isothermal flow**. Click the **Non-isothermal flow** button and enter the name of the temperature variable in the associated edit field if you couple the Weakly Compressible Navier-Stokes application mode to an application mode for heat transfer.

You can use the Non-Isothermal Flow description of the Navier-Stokes equations to describe free convection due to changes in density. In such a case, set the volume force term, $\mathbf{F}$, to the gravity force, $\rho\mathbf{g}$, where $\mathbf{g}$ is a vector that represents the acceleration due to gravity.

The Weakly Compressible Flow Property

You turn on the weakly compressible flow property in the **Application Mode Properties** dialog box, which you open by choosing **Properties** from the **Physics** menu. Set the

Weakly compressible flow property to **On** to use the equations for weakly compressible Navier-Stokes instead of the ones for incompressible Navier-Stokes.

Swirl Flow

The Swirl Flow application mode is an extension of the Incompressible Navier-Stokes application mode for the 2D Axial Symmetry space dimension. The Navier-Stokes in 2D axisymmetry application mode assumes that the azimuthal velocity υ_φ is zero while the Swirl Flow application mode only assumes that there are no variations in any model variable in the azimuthal direction.

For a cylindrical coordinate system, under the assumption that $\partial/\partial\varphi = 0$, Equation 3-5 and Equation 3-6 can be written

$$\frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{\partial u_z}{\partial z} = 0 \tag{3-17}$$

$$\begin{aligned}
\rho\left(\frac{\partial u_r}{\partial t} + u_r\frac{\partial u_r}{\partial r} + u_z\frac{\partial u_r}{\partial z} - \frac{u_\varphi^2}{r}\right) &= -\frac{\partial p}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rr}) + \frac{\partial \tau_{zr}}{\partial z} - \frac{\tau_{\varphi\varphi}}{r} + F_r \\
\rho\left(\frac{\partial u_z}{\partial t} + u_r\frac{\partial u_z}{\partial r} + u_z\frac{\partial u_z}{\partial z}\right) &= -\frac{\partial p}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rz}) + \frac{\partial \tau_{zz}}{\partial z} + F_z \\
\rho\left(\frac{\partial u_\varphi}{\partial t} + u_r\frac{\partial u_\varphi}{\partial r} + \frac{u_r u_\varphi}{r} + u_r\frac{\partial u_\varphi}{\partial z}\right) &= \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\tau_{r\varphi}) + \frac{\partial \tau_{z\varphi}}{\partial z} + F_\varphi
\end{aligned} \tag{3-18}$$

The Newtonian viscous stress tensor in cylindrical coordinates assuming $\partial/\partial\varphi = 0$ is given by

$$\begin{aligned}
\tau_{rr} &= 2\eta\frac{\partial u_r}{\partial r}, & \tau_{zr} = \tau_{rz} &= \eta\left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}\right) \\
\tau_{zz} &= 2\eta\frac{\partial u_z}{\partial z}, & \tau_{r\varphi} = \tau_{\varphi r} &= \eta r\frac{\partial}{\partial r}\left(\frac{u_\varphi}{r}\right) \\
\tau_{\varphi\varphi} &= 2\eta\frac{u_r}{r}, & \tau_{z\varphi} = \tau_{\varphi z} &= \eta\frac{\partial u_\varphi}{\partial z}
\end{aligned}$$

The Swirl Flow application mode uses the notation $u = u_r$, $v = u_z$, and $w = u_\varphi$ and is available for 2D axisymmetric geometries only. COMSOL Multiphysics assumes the symmetry axis to be at $r = 0$. This means that you have to build all models using the axisymmetry modes to the right of the axis $r = 0$. A correctly drawn example is shown in Figure 3-9.

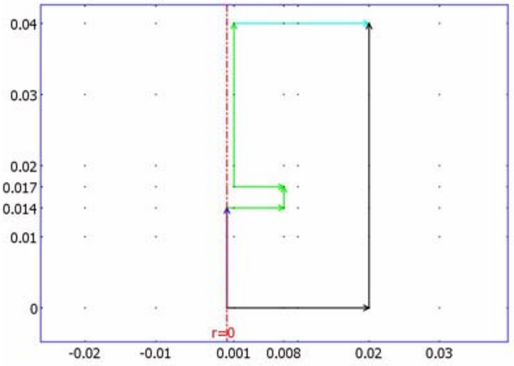


Figure 3-9: A geometry drawn in the 2D Axial Symmetry space dimension. Notice that the whole domain must be contained to the right of the symmetry line $r = 0$.

The Swirl Flow application mode shares boundary conditions, point settings, and artificial diffusion functionality with the Incompressible Navier-Stokes application mode. See "Boundary Conditions" on page 31, "Point Settings" on page 38, and "Numerical Stability—Stabilization Techniques" on page 39. It is also possible to use corner smoothing in the Swirl Flow application mode. See "Corner Smoothing" on page 42.

The Swirl Velocity Property

You turn on the swirl velocity property in the **Application Mode Properties** dialog box, which you open by choosing **Properties** from the **Physics** menu. Set the **Swirl velocity** property to **On** to turn on the swirl flow component and the Swirl Flow application mode for 2D axisymmetric models.

Poroelasticity

Note: The Poroelasticity predefined multiphysics coupling requires the Structural Mechanics Module or the MEMS Module.

Background and Theory

Poroelasticity describes diffusion in elastic solids. Poroelastic models typically describe the linked interaction between fluids and deformation in porous media. For example, the fluids in a reservoir absorb stress, which registers as fluid pressure or equally hydraulic head.

CONSTITUTIVE RELATIONS

Of the two constitutive relations governing poroelastic behavior, one relates stress (total), strain (unambiguous), and pore pressure:

$$\sigma = C\varepsilon - \alpha pI \tag{3-19}$$

The elasticity matrix C must in this formulation be measured under "drained" conditions, that is, by measuring the strain induced by a change in stress under constant pore pressure. Splitting the above relation in a spherical and a deviatoric part, it can be seen that the deviatoric part (shear stresses) are independent of the pore-pressure coupling. The spherical part can be written

$$P = -K\varepsilon_{ii} + \alpha p \tag{3-20}$$

where P is the total mean pressure (positive in compression) and K is the bulk modulus of the drained material.

The other constitutive relation relates an increment in fluid content ζ to volumetric strain and incremental pore pressure:

$$d\zeta = \alpha\varepsilon_{ii} + \frac{dp}{M} \tag{3-21}$$

The empirical constant α is the *Biot-Willis coefficient*, which (as can be seen by setting $dp = 0$) relates the volume of fluid expelled (or sucked into) a material element to the volumetric change of the same element.

The constant M, sometimes called the Biot modulus, is the inverse of the storage coefficient S. It is defined through Equation 3-21 under constant volumetric strain:

$$S = \frac{1}{M} = \left.\frac{\partial\zeta}{\partial p}\right|_{\varepsilon_{ii}} \tag{3-22}$$

Using this definition, it is possible to measure the storage coefficient directly, but at least in the case of an ideal porous material it can be calculated from basic material properties as

$$S = \frac{1}{M} = \frac{\alpha - \phi}{K_s} + \frac{\phi}{K_f} \tag{3-23}$$

Here, ϕ is the porosity, K_f the fluid bulk modulus, and K_s the solid bulk modulus, that is, the would-be bulk modulus of a homogenous block of the material making up the grains. An ideal material is one for which the porosity does not change under a load such that the total normal stress is equal to the pore pressure.

Fluid Flow—Darcy's Law

Darcy's law describes the flow field in the poroelastic model. The fluid equation is

$$S_\alpha\frac{\partial H}{\partial t} + \nabla\cdot[-K\nabla H] = -\alpha_\mathrm{b}\frac{\partial}{\partial t}\varepsilon_\mathrm{vol} \tag{3-24}$$

where $\partial\varepsilon_\mathrm{vol}/\partial t$ is the time rate of change of volumetric strain from the equation for solid displacements; and α_b is the Biot-Willis coefficient. You can interpret the right-hand term as the time rate of expansion of the solid matrix. The volume fraction available for liquid increases and thereby gives rise to liquid sink, which is why the sign is reversed in the source term.

Solids Deformation

Navier's equations for a solid in equilibrium under purely gravitational load is

$$-\nabla\cdot\sigma = \rho_\mathrm{av}\mathbf{g} = (\rho_f\phi + \rho_s(1-\phi))\mathbf{g} \tag{3-25}$$

where σ is the total stress tensor from Equation 3-19 and ρ_av, ρ_f and ρ_s represent average, fluid and solid densities, respectively. 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.

Note that Equation 3-25, which describes an equilibrium state, is used also when the flow model is time-dependent. 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 will change in time—even if Equation 3-25 appears to be stationary—and that the structure-to-fluid coupling term, involving the rate of strain, will be nonzero.

Implementation

The Poroelasticity predefined multiphysics coupling combines a transient formulation of Darcy's law in the Darcy's Law application mode with a quasi-static structural mechanics application mode.

Poroelasticity is available in the following space dimensions:

- In 2D using a plane strain analysis, adding the Plane Strain application mode
- In 2D axisymmetry, the predefined coupling uses the Axial Symmetry, Stress-Strain application mode
- In 3D, the Solid, Stress-Strain application mode describes the elastic solid

In all cases, the predefined multiphysics coupling uses the Darcy's Law application mode in the Earth Science Module, and you can choose to use the interface for pressure (p), pressure head (H_p), or hydraulic head (H). The structural mechanics application mode comes the Structural Mechanics Module or the MEMS Module.

The poroelasticity coupling means that the liquid source in the Darcy's Law includes a default group that sets the liquid source Q_s to the right-hand side in Equation 3-24, which includes the Biot-Willis coefficient α_b, which is a dimensionless coefficient with a default value of 1. You can change its value in the **Biot-Willis coefficient** edit field, which you find in the **Subdomain Settings** dialog box for the Darcy's Law application mode when you start a model using the Poroelasticity predefined multiphysics coupling. Also, the default group activates the gravity effect by setting the **Elevation/ vertical axis** property in the **Application Scalar Variables** dialog box to be the vertical axis (the y-axis in 2D plane strain models, and the z-axis in 2D axisymmetric and 3D models).

In the structural mechanics application mode, default group selects the **Include initial pressure** check box and sets the initial pressure to the second term in the right-hand side of Equation 3-19. It also applies gravity as a volume force (body force) $\boldsymbol{F}$.

The default group also changes the default material properties to approximately representing medium-grained quartz sand using SI units. For the Darcy's Law application mode, the following table lists the default values:

TABLE 3-2: DARCY' LAW: DEFAULT MATERIAL PROPERTIES FOR POROELASTICITY

PROPERTY	VALUE
Storage term	Specific storage
θ_s	0.25
X_f	$4.4\cdot10^{-10}$ 1/Pa
X_p	$2.7\cdot10^{-11}$ 1/Pa
Hydraulic conductivity/Permeability	Permeability
κ_s	$3\cdot10^{-11}$ m^2
ρ	1000 kg/m^3
η	0.001 Pa·s
α_b	1

To keep the default material consistent if you switch between pressure analysis and head analysis, the default settings use the specific storage setting instead of the explicit, user-defined storage term.

The following table show the default material property values for the structural mechanics application mode. The shear modulus and the Poisson number depend on a lot of factors. Therefore, these default values are plausible but cannot be said to represent any particular configuration.

TABLE 3-3: STRUCTURAL MECHANICS: DEFAULT MATERIAL PROPERTIES FOR POROELASTICITY

PROPERTY	VALUE
E	750 MPa
ν	0.25
α	$3.5\cdot10^{-7}$ 1/K
ρ	1915 kg/m^3

To start a model using the Poroelasticity predefined multiphysics coupling, open the **Earth Science Module>Poroelasticity** folder in the Model Navigator, and in 3D, for example, choose one of the following:

- **Stress-Strain, Pressure**
- **Stress-Strain, Pressure head**
- **Stress-Strain, Hydraulic head**

Example Model

The Biot Poroelasticity model on page 201 of the *Earth Science Module Model Library* uses the Poroelasticity multiphysics coupling.

4

Heat Transfer Application Modes

This chapter provides information about the application modes for modeling heat transfer in the Earth Science Module.

Overview

The heat transfer applications in the Earth Science Module characterize temperature distributions for geological phenomena and freely couple to other physics in a model. The application modes apply to systems consisting of solids, fluids, and fluid-solid mixtures. Included are interfaces to calculate effective properties for porous media consisting of a fluid and a solid component, or a rock formation with different mineral proportions. The application modes also feature predefined expressions to represent the geotherm as a radiogenic heat source.

The Conduction application mode 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, or cooling earth analyses. The application mode 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 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.

The Convection and Conduction application mode describes 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. Moving magma is another example. With a moving fluid comes the need to consider how heat spreads; in many cases the fluid moves around solid particles rather than straight through them. Among various methods to describe the spreading, the application mode offers a thermal dispersion tensor analogous to mechanical dispersion in solute transport equations.

These application modes easily combine 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.

Conduction

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. It is responsible for the vast majority of heat transferred within and through the earth's surface. Conductive heat transfers can be long-term steady or exquisitely sensitive over tiny time increments. They can involve molten materials, mineral grains, fluids trapped within interstices, human structures, and molten rock. The heat conduction of heat 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.

The Conduction application mode from the Earth Science 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 application mode 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 Conduction application mode couples, in a straightforward manner, to the convection and conduction application modes as well as any other physics represented in a model file.

Fourier's law describes heat transfer by conduction according to

$$\delta_{\mathrm{ts}} C_{\mathrm{eq}} \frac{\partial T}{\partial t} + \nabla \cdot (-K_{\mathrm{eq}} \nabla T) = Q_H + Q_G + Q_C + Q_R$$

In this equation, temperature (T) is the dependent variable. The volumetric heat capacity, C_{eq}, describes the potential per volume to store heat and so dictates changes in heat stored with time. The thermal conductivity, K_{eq}, characterizes how readily the heat is transmitted. The heat sources and sinks Q_H, Q_G, Q_C, and Q_R, are respectively the general, geothermal, convective, and radiative transfers subsequently described in detail. The term δ_{ts} is an optional coefficient added mostly for user convenience. In COMSOL Multiphysics, you can define all equation coefficients with arbitrary expressions including those that depend on results from other physics and heat equations set up in a model.

Fourier's law of condition

$$\mathbf{N} = -K_{\mathrm{eq}}\nabla T$$

gives the magnitude and direction of the heat flux. The equation states that the flux, **N**, is proportional to the temperature gradient, and K_{eq} prescribes the temperature gradient needed to achieve a given flux.

Effective Thermal Properties

The equation coefficients C_{eq} and K_{eq} are effective properties that describe a representative volume of the solids, liquids, gases in a model to store and transmit heat. Of course, the effective properties can change value in space and time and even depend on results from this equation and others. The volume fraction of a particularly conductive mineral, for example, might vary as mineral abundance changes from one location to the next in the model domain. Moreover, the heat capacity and the thermal conductivity of that mineral might change with temperature or respond to chemical reactions.

As an option, the Earth Science Module automatically defines C_{eq} and K_{eq} with information you provide about the volume fraction, θ, density, ρ, specific heat capacity, C_p, and thermal conductivity, K. You give data for the fluids and solids in a model and how they vary with temperature and reactions, for example. The equations used to define C_{eq} and K_{eq} are

$$C_{\mathrm{eq}} = \frac{\Sigma\theta_{\mathrm{L}i}\rho_{\mathrm{L}i}C_{p\mathrm{L}i} + \Sigma\theta_{\mathrm{P}i}\rho_{\mathrm{P}i}C_{p\mathrm{P}i}}{\Sigma\theta_{\mathrm{L}i} + \Sigma\theta_{\mathrm{P}i}}$$

$$K_{\mathrm{eq}} = \frac{\Sigma\theta_{\mathrm{L}i}K_{\mathrm{L}i} + \Sigma\theta_{\mathrm{P}i}K_{\mathrm{P}i}}{\Sigma\theta_{\mathrm{L}i} + \Sigma\theta_{\mathrm{P}i}}$$

Here the subscripts "L" and "P" denote liquid and solid properties, respectively. The equations amount to volume averaging.

Geothermal Heating

Geothermal temperature gradients are typically on the order of 25 °C per kilometer. Produced by spontaneous decay of the radiogenic materials common in the subsurface, the gradient varies with factors such as rock type, fluid content, and mineral abundance. This application mode introduces the geotherm as a heat source, Q_G, based on the radiogenic decay produced by the rocks, fluids, and gases in a model. By way of contrast, representing the geothermal gradient with boundary conditions complicates heat transfer modeling because of competing conditions on the same point, edge, or face. Typical decay rates and densities for different rock and mineral types appear in Ref. 1 and Ref. 2.

The Conduction application mode predefines uniform and exponential distributions for radiogenic heat sources. You can also define the geotherm according to another rule. For instance, the exponential law (Ref. 1 and Ref. 2) for geothermal heating states

$$Q_G = \rho_{\mathrm{geo}} q_{\mathrm{geo}} e^{\frac{z_{geo}}{h_{geo}}}$$

In this equation, ρ_{geo} is the geothermal density, and q_{geo} is the radiogenic heating per unit mass. The geothermal heating per unit volume, Q_G, varies exponentially along the vertical dimension of the domain, z_{geo}, according to a length scale h_{geo}. Here z_{geo} is a model coordinate x, y, or z. In the Earth Science Module, you can calculate the density, ρ_{geo}, automatically using all or part of the solid and fluid densities catalogs in the materials table.

The uniform geothermal heating law is

$$Q_G = \rho_{\mathrm{geo}} q_{\mathrm{geo}}$$

Accordingly, the model introduces no change in the source strength with depth.

Heat Sources for 1D and 2D Models

In addition to the geothermal heating, Q_G, already described, you can represent a wide variety of heat sources and sinks in a model. The software provides templates for formulating the convective (Q_C) and radiative (Q_R) terms and leaves the general heat source (Q_H) entirely to your discretion.

The convective heat source, Q_C, represents heat transfer in proportion to an external temperature. Typical scenarios include heating and cooling with flowing fluids such as air, water, or magma, and transfer through an overlying but unmodeled layer. The equation for Q_C reads

$$Q_C = h(T_{\mathrm{inf}} - T)$$

With this formulation, the external temperature is T_{inf}, and T is the temperature at the present location. The proportionality term h denotes a heat transfer coefficient, which depends on material properties, the model geometry, and the model physics. For inspiration look to the many tables of h values obtained empirically for various application. The Earth Science Module provides several examples of formulas to arrive at physically based h values.

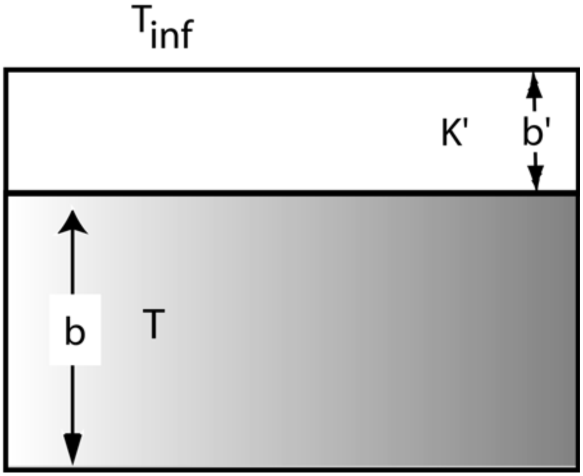
You can describe sensible heat transfer from the soil to some air flowing over the domain as

$$Q_C = h(T_{\mathrm{inf}} - T) = gC_{\mathrm{f}}(T_{\mathrm{inf}} - T)$$

where g is a lumped parameter that includes the fluid velocity, and C_{f} is the volumetric heat capacity of the mobile fluid. The parameter g represents the sensible heating and is

$$g = 2.15 \cdot 10^{-5}\left(\frac{T}{T_{\mathrm{ref}}}\right)^{1.75}$$

For this model, assume $T_{\mathrm{ref}} = 293.15$ K.



A model can include heat transfers across an overlying layer without accounting for the full 3D problem. All you need is the temperature above the upper layer T_{inf} *plus the layer's thermal conductivity* K' *and thickness* b'*. This—along with the conductivity,* K*, and thickness,* b*, within the zone of interest—allows you to predict model temperatures,* T*.*

Frequently heat transmitted through an adjacent or overlying layer, such as a soil horizon, affects temperature in your zone of interest. yet a detailed description of the physics in the overlying layer would add little information of value. For example, consider the 2-layer system in the above figure. The model domain, the lower layer, has a thickness b and lies under a relatively thin soil layer with thermal conductivity K' and thickness b'. Above the thin layer, the temperature is T_{inf}. Assuming that the overlying layer transmits heat according to Fourier's law of conduction but does not store it, you can describe the source term as

$$Q_C = h(T_{\mathrm{inf}} - T) = \frac{K'}{b'b}(T_{\mathrm{inf}} - T)$$

To add impacts of incoming or outgoing radiation at the earth's surface, use the heat source term Q_R

$$Q_R = C_{\mathrm{const}}(T_{\mathrm{amb}}{}^4 - T^4) = \sigma\varepsilon(T_{\mathrm{amb}}{}^4 - T^4)$$

This equation state that radiative heat transfer is proportional to T^4. The proportionality term C_{const} often is defined as the product of the Stefan-Boltzmann constant, σ, and the emissivity of the surface, ε.

Boundary Conditions

The Conduction application mode of the Earth Science Module predefines a number of boundary conditions used in heat transfer modeling. Often you know the temperature, for example, at the ground surface or the core-mantle boundary, which gives the Dirichlet condition

$$T = T_0$$

where the specified temperature, T_0, can be a constant, an expression that depends on time t, or hinge on results from another COMSOL Multiphysics application mode.

Often a model predicts just the temperature change related to a given process, or the zero-temperature condition

$$T = 0$$

You can specify any combination of generalized, radiative, and convective fluxes on the boundary using the condition

$$-\mathbf{n} \cdot (-K_{\mathrm{eq}}\nabla T) = N_0 + \frac{h}{dA}(T_{\mathrm{inf}} - T) + \frac{C_{\mathrm{const}}}{dA}(T_{\mathrm{amb}}{}^4 - T^4)$$

In this equation, $\mathbf{n}$ is the normal to the boundary, and dA represents thickness. Here the generalized flux, N_0, can be an arbitrary expression. The second and third terms on the right side of the flux equation are analogs to, respectively, the convective and radiative source terms for 1D and 2D applications. Dividing by the thickness of the diffusive boundary layer, for example, provides dimensional consistency.

The final predefined boundary conditions represents insulation and symmetry as

$$\mathbf{n} \cdot (K_{\mathrm{eq}} \nabla T) = 0$$

which specifies zero flux perpendicular to the boundary but allows temperatures to change along its length.

References

1. D.L. Turcotte and G. Schubert, *Geodynamics*, Cambridge University Press, 2002.

2. N.H. Sleep and K. Fujita, *Principles of Geophysics*, Blackwell Science Inc., 1997.

Convection and Conduction

This application mode sets up analyses for heat transferred by convection and conduction for earth science applications. With it you can describe heat carried by moving oil, water, magma that you describe with a velocity field. Presumably the velocity is nonzero, but not necessarily so. You can use the Convection and Conduction application mode handles 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 application mode provides a number of options to characterize the geothermal gradient.

To overview the Convection and Conduction application mode, this discussion 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 equation that describes heat transfer by convection and conduction reads

$$\delta_{\mathrm{ts}}\ C_{\mathrm{eq}}\frac{\partial T}{\partial t} + \nabla\cdot(-K_{\mathrm{eq}}\nabla T) = -C_{\mathrm{L}}\mathbf{u}\nabla T + Q_H + Q_G \tag{4-1}$$

The dependent variable is temperature, T. In the equation, C_{eq} denotes the effective volumetric heat capacity; K_{eq} defines the effective thermal conductivity; and C_{L} is the volumetric heat capacity of the moving fluid. The total fluid velocity, $\mathbf{u}$, is a vector of directional velocities u, v, and w for 3D systems. The terms on the right-hand side of the equation, Q_H and Q_G, denote both general and geothermal heat sources. The equation coefficients and source terms can be spatially and temporally varying, remain constant, depend on the temperature T, and link to any other physics in the model.

The heat flux incudes transfers within and between immobile constituents as well as the moving fluid. The total heat flux is the bracketed expression in the governing equation

$$\mathbf{N} = -K_{\mathrm{eq}}\nabla T + C_{\mathrm{L}}\mathbf{u}T$$

where $\mathbf{N}$ denotes the heat flux vector and the temperature, T, is the dependent variable.

This equation for the heat flux vector, **N**, contains two terms. The first describes flux in proportion to the temperature gradient; the second is the convective flux or the heat moving at the liquid's bulk velocity. In a dry solid, heat flux proportional to a temperature gradient describes spreading of heat by atomic vibration or conduction alone. For porous media, however, the spreading might also include small-scale variations in the velocity's magnitude and direction.

Effective Properties

Because the moving liquid occupies only the interstices between solid grains, you can describe the convective transfers to and from a model element with the liquid properties alone. For conduction, it is reasonable to lump the properties of the mobile fluid and the fixed components within a porous medium. In the Earth Science Module you can choose to enter the different materials in a model and automate the calculation of the effective properties as follows.

C_{eq} is the effective property that describes the volumetric capacity to store heat. It typically is defined by volume averaging the storage properties of all constituents in the model element.

K_{eq} describes the rate at which the heat transfers. It accounts for heat transfers by strict conduction or atomic vibration. In addition, some scientists argue that K_{eq}, along with conduction, should account for the mechanical dispersion of heat. In parallel to the dispersion tensor in solute transport, the spreading of heat when moving fluids navigate around solid particles is separate and distinct from convection with the bulk fluid direction. This type of dispersion depends on the fluid velocity as well as the temperature gradient.

Geothermal Heating

The geotherm (the temperature change with depth seen in most geologic settings) results from the spontaneous decay of radiogenic materials that naturally occurs within rocks. The Earth Science Module introduces the geotherm as a volumetric heat source, Q_G. You can define the geotherm using a variety of expressions. Offered are the uniform and the exponential rules set out in Ref. 1 and Ref. 2. Details about these methods appear in the section "Conduction" on page 61.

Boundary Conditions

The Convection and Conduction application mode predefines a number of boundary conditions for earth science applications. To use these predefined set ups to explain how the model domain interacts with the surrounding environment, you fill blanks for the specified temperatures and fluxes with intuitive expressions, results from adjacent domains or other applications. The following boundary conditions are available:

- Temperature: Specify a temperature on the boundary.
- Heat flux: Specify the inward heat flux across the boundary.
- Convective flux: This boundary condition represents a boundary where heat flows in our out with a fluid (that is, heat transfer is dominated by convection).
- Thermal insulation: There is no heat flux across the boundary (the default condition).
- Axial symmetry: Use this boundary condition on the symmetry axis (available in axisymmetric models only).

The fundamental piece of data in many environmental scenarios is a measurement of temperature. You can enter the boundary temperature as a constant, model results, or as a string of data that the software interpolates between the points.

Many geologic processes involve periodic heating and cooling that you can model using the Temperature boundary condition. For example, day-to-night (diurnal) heating produces seasonal variations in temperature as well as long-term fluctuations that explain glaciation episodes. Consider diurnal heating at the ground surface, often described with the following condition:

$$T_0 = \bar{T} + T_A \sin\left(\frac{2\pi t}{t_p} - \frac{7\pi}{12}\right)$$

This equation represents the temperature fluctuation as wave. Here $\overline{T}$ is the average temperature at the ground surface, T_A is the amplitude of the sine wave or the maximum temperature fluctuation, t is the current time, and t_p is the time period (1 day). This equation sets up the maximum temperature at 1:00 PM with the second term in the sine argument.

Often the total heat flux is available or can be deduced, for example, at the ground surface near a volcano or the mid-ocean ridge. Here you define the heat flux N_0 using the third boundary expression in the list.

The convective flux condition, the fourth boundary expression, is a “free” boundary statement because it allows you to solve for the convective flux, setting the conductive portion of the heat flux to zero. This boundary condition applies in situations where the moving fluid carries the vast majority of heat.

The last two predefined boundary equations, the insulation and symmetry conditions, also specify the flux. The statement dictates that zero heat flows across the boundary but allows temperatures to change along it.

Thermal Properties

Modeling convection and conduction in porous media requires effective properties C_{eq} and K_{eq} for a representative volume of the solids, liquids, and gases as well as C_{L}, which describes only the moving fluid. By way of contrast, for free flows, C_{eq} and K_{eq} amount to thermal properties of the moving fluid C_{L} and K_{L}.

This application mode provides tables to enter material properties of each constituent in the porous media and options to calculate C_{eq} and K_{eq}. The individual and lumped parameters can change value in space and time. For instance, the volume fraction of sand might change from 0.9 near a beach to 0.1 inland. The sand’s thermal properties also might change from point to point or vary in time. The application mode provides a table to catalog the volume fraction, θ, the density, ρ, the heat capacity per unit mass or specific heat capacity, C_p, and the thermal conductivity, K, for the mobile and immobile substances in the model domain. As an option, the Earth Science Module automatically defines C_{eq} and K_{eq} on the tabulated data. It also provides edit fields where you can define the effective properties yourself.

VOLUMETRIC HEAT CAPACITY—STORAGE

The volumetric heat capacity, C, denotes the potential for a given volume of a substance to store heat, dictating heat storage changes in time. COMSOL Multiphysics can automatically calculate the effective volumetric heat capacity of the porous medium, C_{eq}, and that of the moving liquid, C_{L}, using the formulae

$$C_{\mathrm{eq}} = \frac{\theta_{\mathrm{L}}\rho_{\mathrm{L}}C_{p\mathrm{L}} + \Sigma\theta_{Gi}\rho_{Gi}C_{pGi} + \Sigma\theta_{Pi}\rho_{Pi}C_{pPi}}{\theta_{\mathrm{L}} + \Sigma\theta_{Gi} + \Sigma\theta_{Pi}}$$

$$C_{\mathrm{L}} = \rho_{\mathrm{L}}\dot{C}_{p\mathrm{L}}$$

Here the subscripts “L,” “G,” and “P” denote the one mobile fluid, the immobile fluids, and solid properties, respectively.

EFFECTIVE THERMAL CONDUCTIVITY—SPREADING

The thermal conductivity, K, describes how readily a substance transmits or spreads heat. The larger K becomes, the smaller the temperature change needed to produce a given heat flux. This application mode provides several methods to define the equivalent thermal conductivity, K_{eq}, and also for you to write your own definition. The predefined options include a power law, a dispersion and conduction approach, and the volume average.

Power Law

With the Power Law method, K_{eq} equals the thermal conductivity of the liquids and solids in a model raised to the power of their volume fractions as in

$$K_{\mathrm{eq}} = K_{\mathrm{L}}^{\theta_L} K_P^{(1-\theta_L)}$$

For a system of water with $K = 0.6$ W/(m·K) and rocks where $K = 2.0$ W/(m·K), the power law predicts *less* spreading of heat (that is, sharper temperature gradients and higher temperatures) than a volume average.

Dispersion and Conduction

In contrast, the conduction and dispersion method Ref. 3 adds spreading from variations in liquid velocity or thermal dispersion, K_{Disp}, to the flux results from atomic vibration (conduction) through the porous medium, K_{PM}.

$$K_{\mathrm{eq}} = K_{\mathrm{PM}} + K_{\mathrm{Disp}}$$

A glance at the equation reveals that the dispersion and conduction method clearly yields more spreading of heat than would conduction alone K_{PM}. Note that K_{PM} typically is defined as a volume average, following the equations given in the previous discussion of the Conduction application mode.

You can choose to define K_{Disp} on your own or automate the definition according to Ref. 3 using fluid velocities with materials information you tabulate. For fluid velocities u, v, and w, corresponding to the x, y, and z directions, the equations are

$$K_{\mathrm{Disp}xx} = \lambda_1 C_{\mathrm{L}}\frac{u^2}{|\mathbf{u}|} + \lambda_2 C_{\mathrm{L}}\frac{v^2}{|\mathbf{u}|} + \lambda_3 C_{\mathrm{L}}\frac{w^2}{|\mathbf{u}|}$$

$$K_{\mathrm{Disp}yy} = \lambda_1 C_{\mathrm{L}}\frac{v^2}{|\mathbf{u}|} + \lambda_2 C_{\mathrm{L}}\frac{u^2}{|\mathbf{u}|} + \lambda_3 C_{\mathrm{L}}\frac{w^2}{|\mathbf{u}|}$$

$$K_{\mathrm{Disp}zz} = \lambda_1 C_{\mathrm{L}}\frac{w^2}{|\mathbf{u}|} + \lambda_3 C_{\mathrm{L}}\frac{u^2}{|\mathbf{u}|} + \lambda_3 C_{\mathrm{L}}\frac{v^2}{|\mathbf{u}|}$$

$$K_{\mathrm{Disp}xy} = K_{\mathrm{Disp}yx} = (\lambda_1 - \lambda_2) C_{\mathrm{L}}\frac{uv}{|\mathbf{u}|}$$

$$K_{\mathrm{Disp}xz} = K_{\mathrm{Disp}zx} = (\lambda_1 - \lambda_3) C_{\mathrm{L}}\frac{uw}{|\mathbf{u}|}$$

$$K_{\mathrm{Disp}yz} = K_{\mathrm{Disp}zy} = (\lambda_1 - \lambda_3) C_{\mathrm{L}}\frac{vw}{|\mathbf{u}|}$$

where $K_{\mathrm{Disp}ii}$ are the principal components of the thermal dispersion tensor, $K_{\mathrm{Disp}ji}$ and D_{Lji} are the cross terms; and λ_1 is the thermal dispersivity in the longitudinal direction. λ_2, and λ_3 are the thermal dispersivities in transverse horizontal and transverse vertical directions. Multiplication by the volumetric heat capacity of the mobile fluid, C_{L}, follows since the mobile carries the heat. The spreading of heat this tensor defines is analogous to hydrodynamic dispersion discussed in the previous sections on solute transport.

Volume Average

You also can define K_{eq} as the volume average thermal conductivity of the components in a model. For example, K_{eq} equals K_{PM} when K_{Disp} is set to zero as in

$$K_{\mathrm{eq}} = K_{\mathrm{PM}} = \frac{\theta_{\mathrm{L}} K_{\mathrm{L}} + \Sigma\theta_{Gi} K_{Gi} + \Sigma\theta_{Pi} K_{Pi}}{\theta_{\mathrm{L}} + \Sigma\theta_{Gi} + \Sigma\theta_{Pi}}$$

Artificial Diffusion

Stabilization is sometimes needed since pure Galerkin discretization is unstable for convectively and/or source-term dominated transport equations. The stabilization methods and their effects on the numerical solution are described in Chapter 17, “Stabilization Techniques,” in the *COMSOL Multiphysics Modeling Guide*.

The Convection and Conduction application mode supports artificial diffusion using the following methods:

- Isotropic diffusion

- Streamline diffusion
- Crosswind diffusion

ISOTROPIC DIFFUSION

Isotropic diffusion is described in the section "Isotropic Diffusion" on page 486 of the *COMSOL Multiphysics Modeling Guide*.

STREAMLINE DIFFUSION

There are three types of streamline diffusion available:

- Anisotropic diffusion is described in "Anisotropic Diffusion" on page 487 in the *COMSOL Multiphysics Modeling Guide*.
- The Petrov-Galerkin streamline diffusion is almost the same as the SUPG method described in Chapter 17, "Stabilization Techniques," of the *COMSOL Multiphysics Modeling Guide*. The only difference is an intrinsic time scale that the method uses. The Convection and Conduction application mode uses the original time scale designed for transport equations dominated by convection (see Ref. 4).

  There is no strict theory on the value of the tuning parameter, $\delta_{\mathrm{sd,\,T}}$, but good rule of thumb is to select $\delta_{\mathrm{sd,\,T}} = 0.5/p$ where p is the order of the basis functions.
- The Petrov-Galerkin/Compensated method uses a modified intrinsic time scale that completely eliminates the streamline diffusion contributions in regions dominated by diffusion (Ref. 4).

  There is no strict theory on the value of the tuning parameter, $\delta_{\mathrm{sd,\,T}}$, but good rule of thumb is to select $\delta_{\mathrm{sd,\,T}} = 0.5/p$ where p is the order of the basis functions.

  The drawback is that this formulation can cause discontinuities and that it introduces additional nonlinearities.

CROSSWIND DIFFUSION

Crosswind diffusion provides extra diffusion in the region of sharp gradients. There are two types of crosswind diffusion available:

- Ordo $h^{3/2}$–The Ordo $h^{3/2}$ crosswind-diffusion algorithm adds a diffusion coefficient according to Ref. 5.

  This method should be used only with linear elements but is computational inexpensive. The constant δ_{cd} is per default set to 0.35. This value is however only valid for SI units and must be recalculated if other physical units are used.
- Shock capturing–The COMSOL Multiphysics implementation adds shock capturing according to:

$$\sum_{e=1}^{N_{el}} \int_{\Omega^e} \frac{1}{2}\alpha_c^e h^e \frac{|\Re(c)|}{|\nabla c|} \nabla\hat{c} \cdot \left(I - \frac{1}{|\mathbf{u}|^2}(\mathbf{u} \otimes \mathbf{u})\right) \cdot \nabla c d\Omega$$

where $\Re(c)$ is the equation residual $(\Re(c) = \nabla\Gamma_c - R)$ and $\hat{c}$ is the test function for c. The effective diffusion coefficient, $\alpha^e{}_c$, is

$$\alpha_c^e = \max(0, \delta_{\mathrm{cd}} - 1/\gamma_p^e)$$

$$\gamma_p^e = \frac{|\mathbf{u}|h^e}{2D}$$

$$\beta_p = \frac{R}{|\nabla c|^2}\nabla c$$

where D is the mean diffusion coefficient and R is the reaction term. The tuning coefficient δ_{cd} is set to 0.35, which correlates to second-order basis functions (see Ref. 6).

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5

Solute Transport Application Modes

This chapter provides information about the application modes for modeling solute transport in the Earth Science Module.

Overview

The solute transport applications in the Earth Science Module describe the movements and reactions of a single solute, multiple solutes, and solutes that interact. The first Solute Transport application model suits modeling of transport in saturated porous media, fluids, and even solid state diffusion. With the mode, the physics can be slow diffusion in a solid or stagnant pond, rapid transport in a fracture, or temperature-dependent reactions in multiple phases. The Variably Saturated Solute Transport application mode covers leaching from pesticide applications and landfills as well as chemical partitioning from liquid to vapor phase.

These equation setups facilitate environmental models of pollutants migrating in an aquifer and reservoir analyses involving oil flow stimulated by surfactants. They also suit assessing microbial communities and movement of dissolved oxygen in a river or waste stream.

Linking arbitrarily to and from other physics 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 file.

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

Solute Transport

Analyzing the fate and transport of chemicals in saturated porous media, in liquids, or in solids often requires assessing multiple interacting processes. Considered for single, multiple, or reacting species in porous media can be advection with moving fluids, dispersion or mechanical mixing, molecular diffusion, sorption to solids, and chemical reactions in and between liquids and solids. Dissolved contaminants or "solutes" can move within interstices in an aquifer or reservoir as well as freely in lakes, wells, or streams. You typically link the fluid velocities to another application mode in your model or set them with mathematical expressions. For example, velocities set to zero gives simple diffusion in a stagnant porous media block, puddle or solid.

The governing equation (Ref. 1) for saturated porous media and entirely fluid or solid systems is

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{Pi}}{\partial c} \frac{\partial c_i}{\partial t} + \nabla \cdot [-\theta_s D_{Li} \nabla c_i + \mathbf{u} c_i] = R_{Li} + R_{Pi} + S_{ci}\,.$$

Here, c_i and c_{Pi} respectively denote the solute concentration in the liquid (mass per liquid volume), and that sorbed to solid particles (mass per dry unit weight of the solid) for species i. In the equation, θ_s (termed porosity) is the volume of fluids divided by the total fluid-solid volume; and $\rho_b = (1 - \theta_s)\rho_p$ is the bulk density of the porous medium when ρ_p is the particle density. D_{Li} represents the hydrodynamic dispersion tensor, and $\mathbf{u}$ is the vector of directional velocities. R_{Li} and R_{Pi} describe reactions in the liquid and solid phases, while S_{ci} denotes a solute source. The various equation coefficients can be arbitrary expressions that, for instance, define kinetics. Likewise, you need not employ all the terms in the governing equation; you can easily set unneeded terms and coefficients to zero.

The first term in the equation gives the time rate change in dissolved mass within the porous medium. The second term represents the time change in solute mass sorbed or attached to solids. The bracketed expression characterizes the solute flux. Within the brackets, the first term describes spreading from mechanical dispersion, which is driven by small-scale variations in velocity in proportion to the concentration gradient. The same term also includes molecular diffusion, which accounts for spreading from a concentration gradient alone. The second term in the brackets gives the advective flux, or the flux associated with the mean flow velocity. On the right-hand side are reactions for the liquid phase, the solid phase, and a solute source. The reactions and sources take on positive values for processes that increases concentrations (sources) and negative values for processes that decrease them (sinks). These reaction and source terms can be expressions representing arbitrary processes including dependencies to other physics.

Advection

Advection describes the movement of a solute, such as a pollutant, with the bulk fluid. For simple cases involving steady flow, you could track the position of a solute plume based on the vector of average linear fluid velocities $\mathbf{u}_a$ as in

$$\mathbf{u}_a = \frac{\mathbf{u}}{\theta_s}$$

where θ_s represents the volume fraction containing the mobile fluid. For free fluids, θ_s equals 1; for porous media, θ_s is saturated porosity typically with values of 0.1 to 0.5.

A porous media block 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.

In the solute transport application modes, you provide the net velocity across a surface (for example, the specific or Darcy velocity $\mathbf{u}$ from the Darcy's Law application mode) rather than the velocity within the pores (for example, the average linear velocity, $\mathbf{u}_a$).

Consider the release of a nonsorbing contaminant to a stream. Initially the center of the contaminant plume is located at point x_0. During travel over the time period Δt, the center of mass reaches point $x_1 = u\ \Delta t$.

By way of contrast, a porous medium consists of a solid fraction $1 - \theta_s$ and a liquid fraction θ_s. The contaminant travels at the average linear velocity within only the pore channels u_a. If the fluids occupy only 10% of the porous medium, the distance that the plume proceeds $u_a \Delta t$ is 10 times further than you would predict using the Darcy velocity for the uninterrupted surface $u\ \Delta t$.

Sorption and Retardation

Certain solutes move from the liquid and attach to solid particles, which slows chemical transport through the porous medium. The sorption properties vary between chemicals, so a plume of multiple contaminants may divide into a number of staggered plumes, each with a different composition (Ref. 2).

Attachment to solids "sorption" and detachment from solids "desorption", respectively, reduces or increases dissolved concentrations. The application mode predefines three relationships to predict the solid concentrations, c_{Pi} from the concentration in the liquid phase, c_i:

$$\begin{array}{lll}
c_P = K_P c & \dfrac{\partial c_P}{\partial c} = \dfrac{\partial}{\partial c}(K_P c) & \text{User defined} \\[2ex]
c_P = K_F c^N & \dfrac{\partial c_P}{\partial c} = N K_F c^{N-1} & \text{Freundlich (Ref. 3)} \\[2ex]
c_P = \dfrac{K_L \bar{s} c}{1 + K_L c} & \dfrac{\partial c_P}{\partial c} = \dfrac{K_L \bar{s}}{1 + K_L c^2} & \text{Langmuir (Ref. 4, Ref. 5)}
\end{array}$$

These predefined expressions are sorption isotherms that describe solid and liquid concentrations. Defined at equilibrium, the switch between liquid and solid phases is instantaneous. In COMSOL Multiphysics, you also can enter arbitrary expressions to define, for example, nonequilibrium and temperature-dependent sorption laws, including those set out by Fetter (Ref. 1) and Bear and Verruijt (Ref. 6).

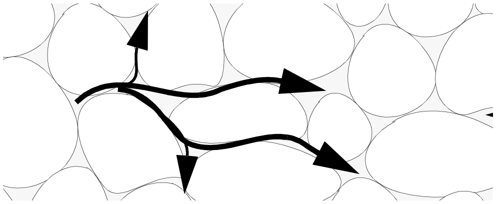
The retardation factor, RF, describes how sorption slows the solute velocity, $\mathbf{u}_c$, relative to the average linear velocity of the fluid, $\mathbf{u}_a$, as in

$$\mathrm{RF} = 1 + \frac{\rho_b}{\theta_s} \frac{\partial c_P}{\partial c} = \frac{\mathbf{u}_a}{\mathbf{u}_c}.$$

If the contaminant moves at the average linear velocity of the fluid for RF = 1. For RF > 1, the contaminant velocity is smaller than the fluid velocity owing to residence time on solids.

Hydrodynamic Dispersion

Hydrodynamic dispersion describes the spreading of contaminant mass. It combines effects from local variations in pore fluid velocity "dispersion" and molecular diffusion. The dispersion occurs because fluids in pore spaces navigate around solid particles, so velocities vary within pore channels (see "Pore-Scale Flow" on page 8 in the *Earth Science Module Model Library*). The spreading in the direction parallel to flow or "longitudinal dispersion" typically exceeds transverse dispersion from 3 to 10 times. Being driven by the concentration gradient alone, molecular diffusion is small relative to the mechanical mixing, except at very low fluid velocities.



Spreading of fluid around solid particles in a porous medium.

The solute transport application modes define hydrodynamic dispersion with the tensor $\theta_s D_{Li}$. For fluid velocities u, v, w corresponding to the x, y, and z directions,

$$\theta_s D_{Lxx} = \alpha_1 \frac{u^2}{|\mathbf{u}|} + \alpha_2 \frac{v^2}{|\mathbf{u}|} + \alpha_3 \frac{w^2}{|\mathbf{u}|} + \theta_s \tau_L D_m$$

$$\theta_s D_{Lyy} = \alpha_1 \frac{v^2}{|\mathbf{u}|} + \alpha_2 \frac{u^2}{|\mathbf{u}|} + \alpha_3 \frac{w^2}{|\mathbf{u}|} + \theta_s \tau_L D_m$$

$$\theta_s D_{Lzz} = \alpha_1 \frac{w^2}{|\mathbf{u}|} + \alpha_3 \frac{u^2}{|\mathbf{u}|} + \alpha_3 \frac{v^2}{|\mathbf{u}|} + \theta_s \tau_L D_m$$

$$\theta_s D_{Lxy} = \theta_s D_{Lyx} = (\alpha_1 - \alpha_2) \frac{uv}{|\mathbf{u}|}$$

$$\theta_s D_{Lxz} = \theta_s D_{Lzx} = (\alpha_1 - \alpha_3) \frac{uw}{|\mathbf{u}|}$$

$$\theta_s D_{Lyz} = \theta_s D_{Lzy} = (\alpha_1 - \alpha_3) \frac{vw}{|\mathbf{u}|}$$

where D_{Lii} are the principal components of the hydrodynamic dispersion tensor, D_{Lji} and D_{Lji} are the cross terms; and α_1 is the dispersivity parallel to the directional velocity. If z is vertical, α_2 and α_3, are the dispersivities in the transverse horizontal and transverse vertical directions, respectively. The general expression where α_1, α_2, α_3

differ comes from Burnett and Frind (Ref. 7). Setting $\alpha_2 = \alpha_3$ gives the expressions shown in Bear (Ref. 8 and Ref. 9). The tensor entries also define molecular diffusion. Here D_m is the molecular diffusion coefficient, and τ_L is the tortuosity factor (less than 1). Multiplication by τ_L, to account for the solids, returns a diffusive flux that is less than that predicted for a strictly liquid system because the solid grains impede the Brownian motion. The application provides options to define $\tau_\mathrm{L} = \theta^{7/3}\,\theta_\mathrm{s}^{-2}$ or to enter arbitrary expressions.

Reactions

Chemical reactions of all types influence solute transport in the environment. The reactions represents change in solute mass per unit volume porous medium per time. Consider, for example, biodegradation, radioactive decay, transformation to tracked products, temperature- and pressure-dependent functions, exothermic reactions, endothermic reactions, and so on. You can use the reaction terms on the right-hand side of the governing equation to represent these processes. For reactions in the fluid phase, multiply the expression by the fluid content θ_s. Similarly, solid phase reaction expressions include bulk density ρ_b. Common examples include

$R_{\mathrm{L}i} = -\theta_s \frac{\ln 2}{\lambda_{Li}} c_i$	Radioactive decay—liquid
$R_{\mathrm{P}i} = -\rho_\mathrm{b} \frac{\ln 2}{\lambda_{\mathrm{P}i}} \left(\frac{\partial c_{Pi}}{\partial c_i}\right) c_i$	Radioactive decay—solid
$R_{\mathrm{L}k} = \theta_s \zeta_{\mathrm{L}i} c_i$	Creation from parent $c_{\mathrm{L}i}$ —liquid
$R_{\mathrm{P}k} = \rho_\mathrm{b} \zeta_{\mathrm{P}i} \left(\frac{\partial c_{\mathrm{P}i}}{\partial c_i}\right) c_i$	Creation from sorbed parent $c_{\mathrm{P}i}$ —solid

where λ is the chemical half life, ζ is a reaction rate, and the subscripts L and P denote liquid and solid phases, respectively. In the equations, the reactions either depend on liquid concentration c_i or solid phase concentrations $c_{\mathrm{P}i}$ obtained using the sorption derivative with c_i.

Reaction rates can vary with results from other equations in your model, such as temperature. For example, you can enter the Arrhenius rate law given in Ref. 4:

$$\zeta_T = \zeta_R \exp\left[\frac{E_\mathrm{a}(T - T_R)}{R_\mathrm{u} T T_R}\right]$$

In this equation, T denotes the current absolute temperature, T_R denotes the reference absolute temperature, E_a is the activation energy, and R_u equals the universal gas constant.

Boundary Conditions

The predefined boundary conditions for solute transport (Ref. 6) follow this paragraph. The first equation is a Dirichlet boundary that sets the concentration to a given value or expression, $c_{i,0}$. The second equation defines the flux with an arbitrary expression, $N_{i,0}$. The third equation sets the flux is zero; in this way, it also represents the condition along an axis of symmetry. Next is a Cauchy condition (General Neumann expression) that states both the concentration and the boundary flux. The Advective flux boundary condition neglects transport by diffusion perpendicular to the boundary. This condition often is described as “free” because it requires specifying neither the flux nor the concentration at an outlet. The Dispersive flux boundary condition specifies a dispersive (diffusive) flux.

$$c_i = c_{i,0} \qquad \text{Concentration}$$
$$\mathbf{n}\cdot(\theta_s D_{\mathrm{L}i}\nabla c_i - \mathbf{u}c_i) = N_{i,0} \qquad \text{Flux}$$
$$\mathbf{n}\cdot(\theta_s D_{\mathrm{L}i}\nabla c_i - \mathbf{u}c_i) = 0 \qquad \text{No flux}$$
$$\mathbf{n}\cdot(\theta_s D_{\mathrm{L}i}\nabla c_i - \mathbf{u}c_i) = \mathbf{n}\cdot\mathbf{u}c_{i,0} + N_{i,0} \qquad \text{General}$$
$$\mathbf{n}\cdot(\theta_s D_{\mathrm{L}i}\nabla c_i) = 0 \qquad \text{Advective flux}$$
$$\mathbf{n}\cdot(\theta_s D_{\mathrm{L}i}\nabla c_i) = N_{i,0} \qquad \text{Dispersive flux}$$

For 2D axisymmetric models, an Axial symmetry boundary condition is available for use on boundaries that represent the axial symmetry axis ($r = 0$). On interior boundaries and pair boundaries, the default boundary condition is Continuity, which provides continuity in the normal flux across the boundary. There is also a Flux discontinuity condition, which specifies a flux discontinuity. The Advective flux, Dispersive flux, and General Neumann expression boundary conditions are also available on interior boundaries and pair boundaries.

Conservative and Nonconservative Formulations

The solute transport application modes in the Earth Science Module are available in conservative and nonconservative formulations. The conservative form of the governing equation

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{Pi}}{\partial c} \frac{\partial c_i}{\partial t} + \nabla \cdot [-\theta_s D_{Li} \nabla c_i + \mathbf{u} c_i] = R_{Li} + R_{Pi} + S_{ci}$$

suits compressible fluids, in which density varies spatially.

The nonconservative form

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{Pi}}{\partial c} \frac{\partial c_i}{\partial t} + \nabla \cdot (-\theta_s D_{Li} \nabla c_i) = -\mathbf{u} \cdot \nabla c_i + R_{Li} + R_{Pi} + S_{ci}$$

is valid for incompressible fluids. In this equation the advective term appears on the right-hand side because the divergence of the velocity vector for an incompressible fluid is zero.

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Variably Saturated Solute Transport

The Variably Saturated Solute Transport application mode describes chemical movement between the liquid, solid, and gas phases in variably saturated porous media. It applies to one or more chemicals that move primarily within a liquid that partially fills the voids in a porous medium. The pore space not filled with liquid contains a relatively immobile gas phase, typically air. For example, pesticides applied at the ground surface leach with irrigation water into dry soil. As it would in saturated porous media, the chemical plume can spread or disperse as the contaminated liquid migrates around solid grains. The chemicals also can diffuse in the water or soil air, adsorb to solids, and react within liquid, solid, or gas.

The system of equations set up here explicitly represents dispersion, advection, sorption, volatilization, and decay for one or more chemicals within variably saturated porous media. You can determine the fluid velocities, the change in liquid fraction with time, and any equation coefficients using predefined expressions, another application mode in your model, or arbitrary mathematical expressions.

The governing equation for chemical transport in variably saturated porous media is

$$\frac{\partial}{\partial t}(\theta c)+\frac{\partial}{\partial t}(\rho_{\mathrm{b}} c_{\mathrm{P}})+\frac{\partial}{\partial t}(a_{\mathrm{v}} c_{\mathrm{G}})+\nabla\cdot[-\theta D_{\mathrm{LG}}\nabla c+\mathbf{u}c] = R_{\mathrm{L}}+R_{\mathrm{P}}+R_{\mathrm{G}}+S_{ci}$$

Here, c, c_{P}, and c_G respectively denote the concentration in the liquid (mass per liquid volume), adsorbed to solid particles (mass per dry unit weight of the solid), and in the gas for a given species i. The equation balances chemical transport throughout the porous medium using the liquid volume fraction θ, the bulk density ρ_{b} and the gas volume fraction a_{v}. The liquid-gas hydrodynamic dispersion tensor D_{LG} and the vector of directional velocities, $\mathbf{u}$, determine where the chemical moves and diffuses. Included in D_{LG} are mechanical spreading from the liquid moving around solid particles, molecular diffusion in the liquid, and volatilization to the gas phase. Reactions in the liquid, solid, and gas phases are R_{L}, R_{P}, and R_{G}. Other solute sources S_{ci} denote concentrations c_q of incoming or outgoing liquids Q_{s} plus arbitrary sources of dissolved solutes S_{o}.

The first group of terms in the governing equation give the time rate change in chemical mass within the porous medium. The bracketed expression characterizes the solute flux. Within the brackets, the first term describes spreading from mechanical dispersion as well as molecular diffusion in the liquid and the gas phase. The second term in the brackets gives the advective flux, or the flux associated with the mean flow velocity. On the right-hand side are reactions for the liquid phase, the solid phase, and a solute source. The reactions and sources take on positive values for processes that increase concentrations (sources) and negative values for processes that decrease them (sinks). These reaction and source terms can be expressions representing arbitrary processes including dependencies to other physics.

The time-dependent terms in the governing equation denote the time rate change in mass within the liquid, solid, and gas phases. Since the concentrations sorbed to solids c_{P} and the gas-phase concentration c_{G} are functions of the liquid-phase concentration, c, you solve for c and calculate c_P and c_G. Expanding the time-dependent terms gives:

$$\frac{\partial}{\partial t}(\theta c)+\frac{\partial}{\partial t}(\rho_{\mathrm{b}}c_{\mathrm{P}})+\frac{\partial}{\partial t}(a_{\mathrm{v}}c_{\mathrm{G}}) = \theta\frac{\partial c}{\partial t}+\rho_{\mathrm{b}}k_{\mathrm{p}}\frac{\partial c}{\partial t}+a_{\mathrm{v}}k_{\mathrm{G}}\frac{\partial c}{\partial t}+(1-k_{\mathrm{G}})c\frac{\partial\theta}{\partial t}$$

Here, the liquid-to-solid and liquid-to-gas partitioning are governed by the sorption isotherm $k_{\mathrm{P}} = \partial c_{\mathrm{P}}/\partial c$ and volatilization isotherm $k_{\mathrm{G}} = \partial c_{\mathrm{G}}/\partial c$. The air volume, a_{v}, is the empty portion of the total porosity θ_s, so it varies as the liquid volume fraction changes $a_{\mathrm{v}} = \theta_{\mathrm{s}} - \theta$.

The solute transport equations for variably saturated porous media differ little from the equations set out for saturated systems described in “Solute Transport” on page 77. The following describes only the changes and new terms needed to account for the partial filling of the pore space as well as transfers to and from the immobile gas phase.

Advection

In solute transport, fluid velocities influence the advection and the dispersion of the chemical. In variably saturated porous media, the vector of average linear fluid velocities, $\mathbf{u}_{\mathrm{a}}$, is given by:

$$\mathbf{u}_{\mathrm{a}} = \frac{\mathbf{u}}{\theta}$$

where the specific velocity, $\mathbf{u}$, describes the net value over surface made up of liquid, solid, and gas. In variably saturated systems, you divide by the liquid volume fraction θ (less than 1) to describe how fast the liquid moves.

Sorption and Retardation

The variably saturated solute transport application accounts for chemical attachment to solids or "sorption." As for saturated porous media, this application mode predefines three sorption relationships:

$$c_\mathrm{P} = K_\mathrm{F} c^N \qquad \frac{\partial c_\mathrm{P}}{\partial c} = N K_\mathrm{F} c^{N-1} \qquad \text{Freundlich}$$

$$c_\mathrm{P} = \frac{K_\mathrm{L} \bar{s} c}{1 + K_\mathrm{L} c} \qquad \frac{\partial c_\mathrm{P}}{\partial c} = \frac{K_\mathrm{L} \bar{s}}{1 + K_\mathrm{L} c^2} \qquad \text{Langmuir}$$

$$c_\mathrm{P} = K_\mathrm{P} c \qquad \frac{\partial c_\mathrm{P}}{\partial c} = \frac{\partial (K_\mathrm{P} c_\mathrm{P})}{\partial c} \qquad \text{User defined}$$

In these equations, the partial derivatives describe the relationship between c_i and $c_{\mathrm{P}i}$ at equilibrium. In COMSOL Multiphysics you also can enter arbitrary expressions to define, for example, nonequilibrium and temperature-dependent sorption laws.

With variably saturated systems, sorption slows the solute velocity, $\mathbf{u}_c$, relative to the fluid velocity, $\mathbf{u}_\mathrm{a}$, which now varies with the liquid content. The retardation factor, **RF** becomes:

$$\mathbf{RF} = 1 + \frac{\rho_\mathrm{b}}{\theta} \frac{\partial c_\mathrm{P}}{\partial c} = \frac{|\mathbf{u}_\mathrm{a}|}{|\mathbf{u}_c|}$$

As discussed for saturated solute transport, the contaminant moves at the average linear velocity of the fluid for $\mathbf{RF} = 1$. For $\mathbf{RF} > 1$, the contaminant moves more slowly than the fluid due to time spent on solids.

Hydrodynamic Dispersion

Hydrodynamic dispersion describes the spreading of contaminant mass due to local variations in pore fluid velocity or "dispersion" and molecular diffusion. In variably saturated porous media, the diffusion in the liquid and the gas phases proceeds according to the concentration gradient. The entries in the liquid-gas dispersion tensor a 2D system are:

$$\theta D_{\mathrm{LG}ii} = \alpha_1 \frac{u_i^2}{|\mathbf{u}|} + \alpha_2 \frac{u_j^2}{|\mathbf{u}|} + \theta D_\mathrm{m} \tau_\mathrm{L} + a_\mathrm{v} D_\mathrm{G} k_\mathrm{G} \tau_\mathrm{G}$$

$$\theta D_{\mathrm{LG}ij} = \theta D_{\mathrm{LG}ji} = (\alpha_1 - \alpha_2)\frac{u_i u_j}{|\mathbf{u}|}.$$

In these equation, $D_{\mathrm{LG}ii}$ are the principal components of the liquid-gas dispersion tensor; $D_{\mathrm{LG}ji}$ and $D_{\mathrm{LG}ji}$ are the cross terms; α is the dispersivity where the subscripts "1" and "2" denote longitudinal and transverse flow, respectively. D_m and D_G are molecular diffusion with tortuosity factors τ_L and τ_G for liquid (water) and gas (air), respectively. The application mode provides options to define $\tau_\mathrm{L} = \theta^{7/3}\theta_\mathrm{s}^{-2}$ and $\tau_\mathrm{G} = a_\mathrm{v}^{7/3}\,\theta_\mathrm{s}^{-2}$ or enter arbitrary expressions.

Reactions

Chemical reactions in variably saturated media can involve processes in the gas phase. For example, common reactions include:

$R_\mathrm{G} = -\frac{\ln 2}{\lambda_{Gi}} a_\mathrm{v}\left(\frac{\partial c_\mathrm{G}}{\partial c}\right)c$	Radioactive decay—gas
$R_\mathrm{G} = -\zeta a_\mathrm{v}\left(\frac{\partial c_\mathrm{G}}{\partial c}\right)c$	Reaction—gas

where λ is the chemical half life and ζ is a reaction rate. The change in gas-phase concentrations c_G depends on the fractional air volume, the volatilization isotherm, and the liquid concentration.

The dissolved and solid-phase reactions listed for saturated porous media in the previous section also apply to variably saturated transport. However, concentrations in the fluid phase now depend on the volume liquid fraction θ instead of the total porosity θ_s. For example,

$R_\mathrm{L} = -\theta\frac{\ln 2}{\lambda_{\mathrm{L}i}} c_i$	Radioactive decay—liquid
$R_\mathrm{L} = -\theta\zeta_\mathrm{L} c_i$	Reaction—liquid

Boundary Conditions

In variably saturated porous media new boundary conditions describe interactions with adjacent gas phases. You can use the no-flow boundary volatilization condition to model only gas-phase diffusion across a boundary. This applies to a no-flow soil surface at the contact with the atmosphere. The boundary condition reads

$$-\mathbf{n}\cdot(-\theta D_{\mathrm{LG}}\nabla c) = \frac{D_{\mathrm{mG}}}{d}k_{\mathrm{G}}(c-c_{\mathrm{atm}}) \qquad \text{No flow volatilization}$$

where d is the thickness of the stagnant boundary layer and c_{atm} is the chemical concentration beyond the stagnant layer.

To account for the concentration of exiting fluid flow in addition to volatilization across the boundary, apply the flow boundary volatilization condition

$$-\mathbf{n}\cdot(-\theta D_{\mathrm{LG}}\nabla c + \mathbf{u}c) = -\mathbf{n}\cdot\mathbf{u}c_0 - \frac{D_{\mathrm{mG}}}{d}k_{\mathrm{G}}(c-c_{\mathrm{atm}}) \qquad \text{Flow volatilization}$$

where the value of c_0 specifies the concentration of the exiting liquid.

Other boundary conditions are virtually identical to those offered for saturated porous media. You can set the concentration or flux to a given value or expression, c_0 and N_0, respectively. You also can set the total flux to zero along a boundary or axis of symmetry. The Cauchy condition states both the concentration and the boundary flux. The advective-flux boundary condition neglects transport by diffusion perpendicular to the boundary. It can be described as “free” because requires specifying neither the flux or the concentration.

$c = c_0$	Concentration
$\mathbf{n}\cdot(\theta D_{\mathrm{LG}}\nabla c - \mathbf{u}c) = N_0$	Flux
$\mathbf{n}\cdot(\theta D_{\mathrm{LG}}\nabla c - \mathbf{u}c) = 0$	No flux/Symmetry
$\mathbf{n}\cdot(\theta D_{\mathrm{LG}}\nabla c - \mathbf{u}c) = \mathbf{n}\cdot\mathbf{u}c_0 + N_0$	General Neumann expression
$\mathbf{n}\cdot(\theta D_{\mathrm{LG}}\nabla c) = 0$	Advective flux
$\mathbf{n}\cdot(\theta D_{\mathrm{LG}}\nabla c) = N_0$	Dispersive flux

Conservative and Nonconservative Formulations

The solute transport application modes in the Earth Science Module are available in conservative and nonconservative formulations. The conservative form of the governing equation

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_{\mathrm{b}}c_{\mathrm{P}}) + \frac{\partial}{\partial t}(a_{\mathrm{v}}c_{\mathrm{G}}) + \nabla\cdot[-\theta D_{\mathrm{LG}}\nabla c + \mathbf{u}c] = R_{\mathrm{L}} + R_{\mathrm{P}} + R_{\mathrm{G}} + S_{ci}$$

suits compressible fluids, in which density varies spatially. The nonconservative form

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_b c_P) + \frac{\partial}{\partial t}(a_v c_G) + \nabla \cdot (-\theta D_{LG} \nabla c) = -\mathbf{u}c + R_L + R_P + R_G + S_{ci}$$

is valid for incompressible fluids. In this equation the advective term appears on the right because the divergence of the velocity vector for an incompressible fluid is zero.

References

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6

Using the Material Libraries

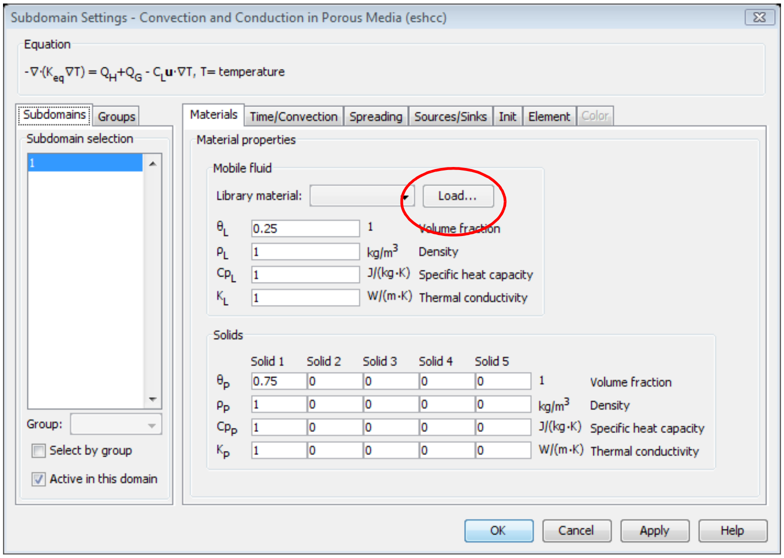
The Materials/Coefficients Library contains an extensive set of mechanical and heat transfer properties for solid materials. In addition, it contains a limited set of fluid properties, which can be used mainly for the fluid-flow and heat transfer application modes.

Material Libraries

A useful feature in COMSOL Multiphysics is the Materials/Coefficients library. The Earth Science Module extends this library with an extra material library, the Liquids and Gases library, with temperature-dependent fluid dynamic and thermal properties.

Loading Material Properties from the Library

For most application modes in COMSOL Multiphysics, you can load a material and its accompanying properties directly from within the **Subdomain Settings** dialog box. First click the **Load** button as indicated in Figure 6-1.



$-\nabla\cdot(K_{eq}\nabla T) = Q_H+Q_G - C_L\mathbf{u}\cdot\nabla T$, T= temperature

Subdomain selection: 1

☐ Select by group

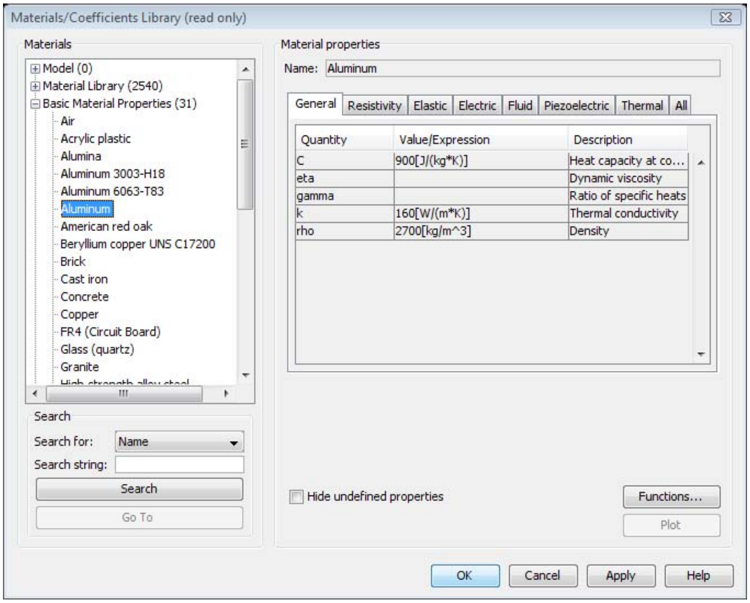
☑ Active in this domain

θ_L	0.25	1	Volume fraction
ρ_L	1	kg/m^3	Density
Cp_L	1	J/(kg·K)	Specific heat capacity
K_L	1	W/(m·K)	Thermal conductivity

	Solid 1	Solid 2	Solid 3	Solid 4	Solid 5		
θ_P	0.75	0	0	0	0	1	Volume fraction
ρ_P	1	0	0	0	0	kg/m^3	Density
Cp_P	1	0	0	0	0	J/(kg·K)	Specific heat capacity
K_P	1	0	0	0	0	W/(m·K)	Thermal conductivity

Figure 6-1: The Load button associated with library materials in the Subdomain Settings dialog box.

This action opens the **Materials/Coefficients Library** dialog box (see Figure 6-2). From there you can select a material to load.



Name: Aluminum

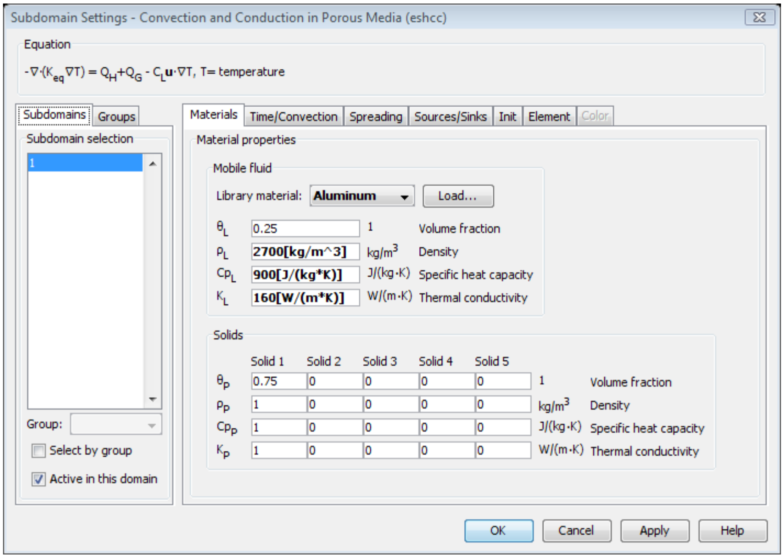
Search for: Name

Quantity	Value/Expression	Description
C	900[J/(kg*K)]	Heat capacity at co...
eta		Dynamic viscosity
gamma		Ratio of specific heats
k	160[W/(m*K)]	Thermal conductivity
rho	2700[kg/m^3]	Density

Figure 6-2: The Materials/Coefficients Library dialog box.

The **Materials** list on the left side contains the installed library folders plus a model folder that contains already-selected materials and coefficients. To load a material into the **Model** folder, select it from the **Materials** list and click **Apply** or **OK**; it now appears in the **Model** folder, which shows all the materials available for the model.

After clicking **OK**, the **Materials/Coefficients Library** dialog box closes and you return to the **Subdomain Settings** dialog box. Now the software has loaded the selected material properties into the corresponding edit fields of that dialog box. The edit fields that contain data taken from the materials library you just selected appear in bold (see Figure 6-3).



Equation

$-\nabla\cdot(K_{eq}\nabla T) = Q_H+Q_G - C_L\mathbf{u}\cdot\nabla T$, T= temperature

Subdomain selection: 1

Group:

☐ Select by group

☑ Active in this domain

Material properties

Mobile fluid

Library material: **Aluminum**

θ_L	0.25	1	Volume fraction
ρ_L	**2700[kg/m^3]**	kg/m^3	Density
Cp_L	**900[J/(kg*K)]**	J/(kg·K)	Specific heat capacity
K_L	**160[W/(m*K)]**	W/(m·K)	Thermal conductivity

Solids

	Solid 1	Solid 2	Solid 3	Solid 4	Solid 5		
θ_P	0.75	0	0	0	0	1	Volume fraction
ρ_P	1	0	0	0	0	kg/m^3	Density
Cp_P	1	0	0	0	0	J/(kg·K)	Specific heat capacity
K_P	1	0	0	0	0	W/(m·K)	Thermal conductivity

Figure 6-3: The Subdomain Settings dialog box after loading aluminum from the material library. Boldface characters indicate that the library material is active.

The Material Libraries

As noted earlier, the **Materials** list in the **Materials/Coefficients Library** dialog box contains multiple expandable folders. The list includes **Model**, **Basic Material Properties**, and additional libraries depending on the modules that your license includes.

Also, if your license includes the COMSOL Material Library, this also appears as a separate folder in the **Materials** list.

Note: The COMSOL Material Library is a separate add-on product that includes over 2500 materials and about 20,000 properties, most of which are temperature-dependent functions.

The Liquids and Gases Library and Material Property Functions

In many cases of modeling the material properties varies with the dependent variables describing the state (temperature, pressure, concentration, potential, stress, and so on). COMSOL Multiphysics is capable of describing material properties as functions of the dependent variables. The following discussion exemplifies use and access a library with material property functions (in this case Liquids and Gases), and also how to edit it and create your own material property functions.

The Liquids and Gases material library contains thermal and fluid dynamic properties for a set of common fluids. All properties are given as functions of temperature and at atmospheric pressure, except the density, which for gases is also a function of the local pressure. The library also contains surface and interface tensions for a selected set of liquid/gas and liquid/liquid systems. All functions are based on data collected from scientific publications. The literature references are noted in the text file `fluids_lib.txt`, located in the data folder of your local COMSOL installation.

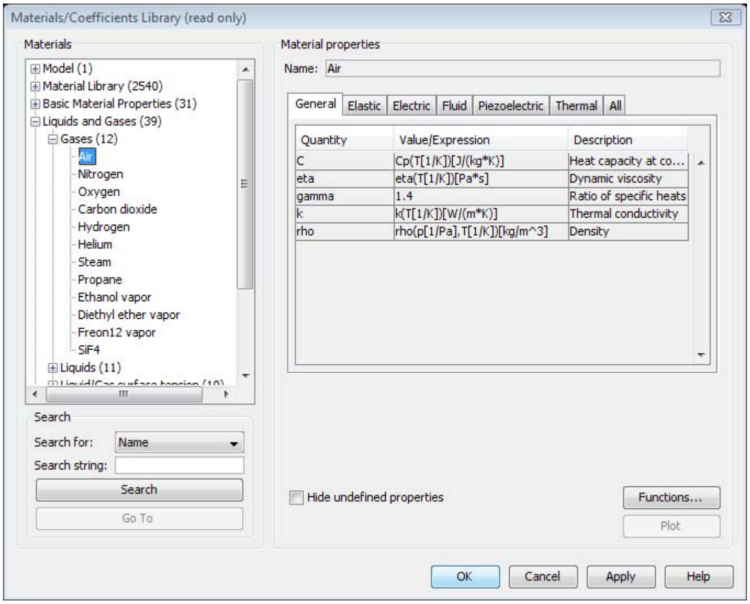
If you click the **Load** button in the **Subdomain Settings** dialog box of any application mode and select to expand **Liquids and Gases** you can choose from various fluids, both liquids or gases (as depicted in Figure 6-4).Their properties are described at atmospheric pressure conditions.

Using Material Property Functions

In many modeling situations, the material properties vary with the dependent variables describing the state (temperature, pressure, concentration, potential, stress, and so on). In COMSOL Multiphysics you can describe material properties as functions of the dependent variables. The following discussion exemplifies how to use a library with material property functions (in this case Liquids and Gases), and also how to edit it and create your own material property functions.

Note: The data-fitted functions expect temperature and pressure arguments to be expressed in the SI units *kelvin* (K) and *pascal* (Pa), respectively, and return values in appropriate SI units. Unit expressions are automatically inserted to handle the conversions to and from the model's base unit system.

If you click the **Load** button in the **Subdomain Settings** dialog box of any application mode and select to expand **Liquids and Gases** you can choose from various fluids, both liquids and gases (see Figure 6-4).



Name: Air

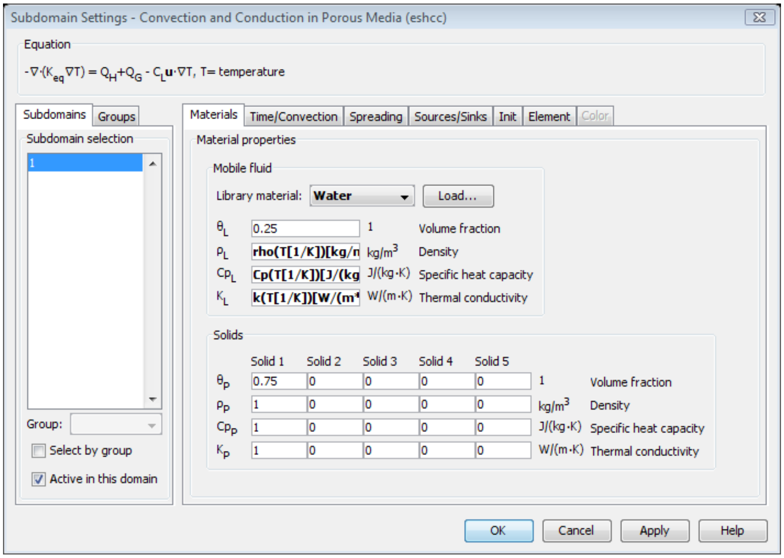
Search for: Name

Quantity	Value/Expression	Description
C	Cp(T[1/K])[J/(kg*K)]	Heat capacity at co...
eta	eta(T[1/K])[Pa*s]	Dynamic viscosity
gamma	1.4	Ratio of specific heats
k	k(T[1/K])[W/(m*K)]	Thermal conductivity
rho	rho(p[1/Pa],T[1/K])[kg/m^3]	Density

☐ Hide undefined properties

Figure 6-4: The Materials/Coefficients Library dialog box, with Liquids and Gases expanded.

If you load a material that uses a function such as those in the Liquids and Gases library, the **Subdomain Settings** dialog box looks like Figure 6-5, with function calls in the edit fields for the material properties.



Equation: $-\nabla\cdot(K_{eq}\nabla T) = Q_H+Q_G - C_L\mathbf{u}\cdot\nabla T$, T= temperature

Subdomain selection: 1

☐ Select by group

☑ Active in this domain

Library material: **Water**

θ_L	0.25	1	Volume fraction
ρ_L	**rho(T[1/K])[kg/n**	kg/m^3	Density
Cp_L	**Cp(T[1/K])[J/(kg**	J/(kg·K)	Specific heat capacity
k_L	**k(T[1/K])[W/(m'**	W/(m·K)	Thermal conductivity

	Solid 1	Solid 2	Solid 3	Solid 4	Solid 5		
θ_p	0.75	0	0	0	0	1	Volume fraction
ρ_p	1	0	0	0	0	kg/m^3	Density
Cp_p	1	0	0	0	0	J/(kg·K)	Specific heat capacity
k_p	1	0	0	0	0	W/(m·K)	Thermal conductivity

Figure 6-5: The Subdomain Settings dialog box after loading a material that uses function calls, for example, the materials from the fluid library.

In this example, the software specifies the material property for density with the function call

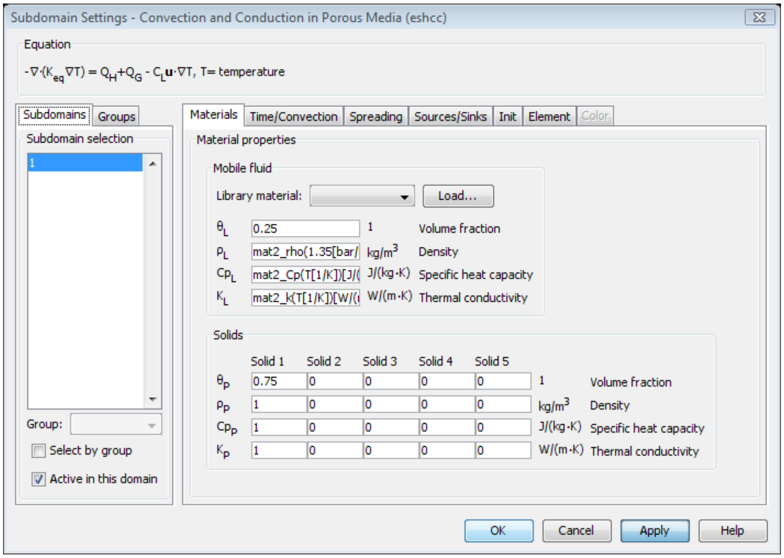
```
rho(p[1/Pa],T[1/K])[kg/m^3]
```

which is a function call to the material loaded, in this case **Water**. The function uses two inputs: pressure, `p`, and temperature, `T`. The default settings are based on the assumption that the temperature variable in the model is `T` and that there is a pressure variable named `p`. Being dependent variables, these are expressed in the model's selected base unit system. The unit expressions inside the function calls convert the values from the model's unit system to nondimensional numbers corresponding to SI units, while the expression between the last brackets makes sure the returned SI value is interpreted correctly in the model's unit system.

In many cases you must change these function inputs. For example, if you model only heat transfer, there is no variable for pressure. In that case you must either specify the pressure directly in the function input or set up a constant or expression for the variable

p. This constant or expression variable must have the dimension of pressure, which you achieve by adding a pressure unit to the expression, such as `135[kPa]`.

It is easy to alter the function input values and variables: simply click inside the parentheses delimiting the function argument and replace the default symbol with the desired value or variable. In the following figure you can see such a modification where a numerical value replaces the pressure variable.



Equation

$-\nabla\cdot(K_{eq}\nabla T) = Q_H+Q_G - C_L\mathbf{u}\cdot\nabla T$, T= temperature

Subdomain selection: 1

Group:

☐ Select by group

☑ Active in this domain

Material properties

Mobile fluid

Library material: Load...

θ_L	0.25	1	Volume fraction
ρ_L	mat2_rho(1.35[bar/	kg/m³	Density
Cp_L	mat2_Cp(T[1/K])[J/(	J/(kg·K)	Specific heat capacity
k_L	mat2_k(T[1/K])[W/(	W/(m·K)	Thermal conductivity

Solids

	Solid 1	Solid 2	Solid 3	Solid 4	Solid 5		
θ_P	0.75	0	0	0	0	1	Volume fraction
ρ_P	1	0	0	0	0	kg/m³	Density
Cp_P	1	0	0	0	0	J/(kg·K)	Specific heat capacity
k_P	1	0	0	0	0	W/(m·K)	Thermal conductivity

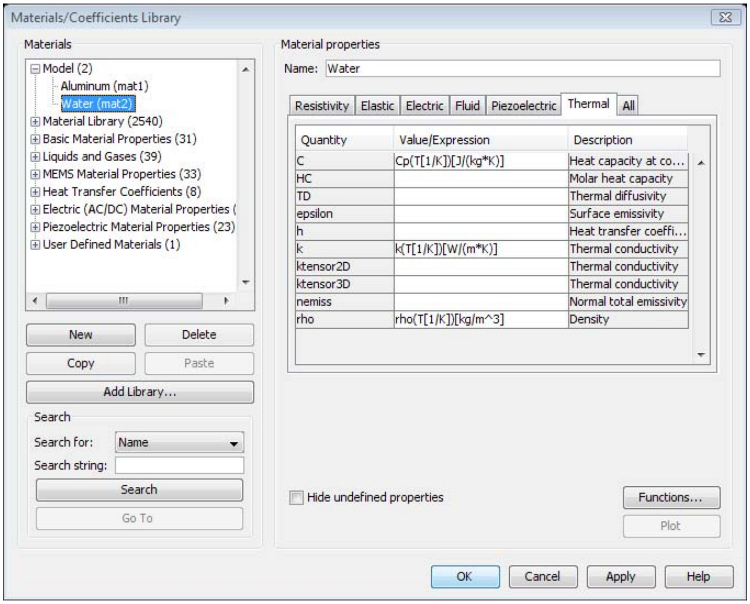
Figure 6-6: Modifying the function inputs. Notice how the unit syntax can convert argument values from any pressure unit to pascal.

In this case the function output is the density for water at the specified pressure and at the temperature given by the variable `T`.

Note: If you override one property defined by a library material by changing anything outside the function arguments, all other property expressions loose their connection to the material library. In particular, material functions appearing in other edit fields (now in plain text instead of in boldface) stop working. The proper way to edit one property of a loaded material is to change the material functions, as described later in this section, rather than editing the edit field in the **Subdomain Settings** dialog box.

USING MATERIAL PROPERTY FUNCTION CALLS OUTSIDE THE SUBDOMAIN SETTINGS

You can also use a library material property function in a model in places other than the **Subdomain Settings** dialog box. One example might be to combine several properties in an expression in the **Scalar Expressions** dialog box. To do so, you must first load the library material into the model using the **Materials/Coefficients Library** dialog box. This dialog box opens either, as described above, from the **Subdomain Settings** dialog box (then in read-only mode), or directly from the **Options** menu. The currently loaded materials and their assigned names are listed in the **Model** folder in the **Materials** tree. (Figure 6-7).



Search for: Name

Name: Water

Quantity	Value/Expression	Description
C	Cp(T[1/K])[J/(kg*K)]	Heat capacity at co...
HC		Molar heat capacity
TD		Thermal diffusivity
epsilon		Surface emissivity
h		Heat transfer coeffi...
k	k(T[1/K])[W/(m*K)]	Thermal conductivity
ktensor2D		Thermal conductivity
ktensor3D		Thermal conductivity
nemiss		Normal total emissivity
rho	rho(T[1/K])[kg/m^3]	Density

Figure 6-7: Viewing the materials loaded into a model along with their names in COMSOL Multiphysics.

In the above figure, two materials are already loaded into the model. COMSOL Multiphysics allocates local material names on the form `matX`, where `X` is a running number assigned in the order in which materials were loaded into the model. In this case, the user loaded **Aluminum** first, so it takes the name `mat1`.

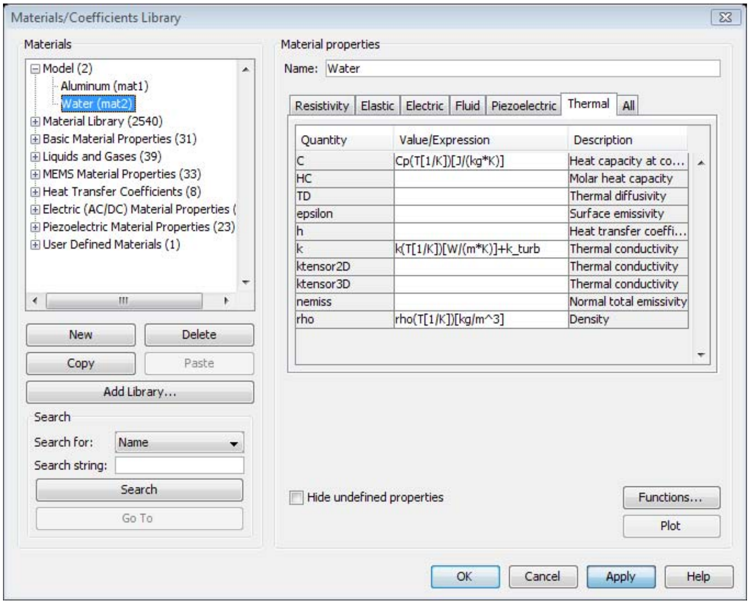
To use a particular material-property function, you can start by copying the syntax shown in the **Value/Expression** column in the **Materials/Coefficients Library** dialog box.

Then you must add `matX_` in front of the function call. Thus, referring to Figure 6-7, to evaluate the function for thermal conductivity of air at 350 K, the syntax is

```
mat2_k(350)[W/m*K]
```

Editing Material Properties

To change a property of a loaded material, choose **Materials/Coefficients Library** from the **Options** menu. This opens the dialog box in edit mode. Then select the desired material in the **Materials** list, click the **Value/Expression** field of interest, and change the expression as depicted in Figure 6-8. In this example the user is adding `k_turb` to the original function for thermal conductivity, where `k_turb` is a variable that must be defined elsewhere in the model.



Name: Water

Quantity	Value/Expression	Description
C	Cp(T[1/K])[J/(kg*K)]	Heat capacity at co...
HC		Molar heat capacity
TD		Thermal diffusivity
epsilon		Surface emissivity
h		Heat transfer coeffi...
k	k(T[1/K])[W/(m*K)]+k_turb	Thermal conductivity
ktensor2D		Thermal conductivity
ktensor3D		Thermal conductivity
nemiss		Normal total emissivity
rho	rho(T[1/K])[kg/m^3]	Density

Search for: Name

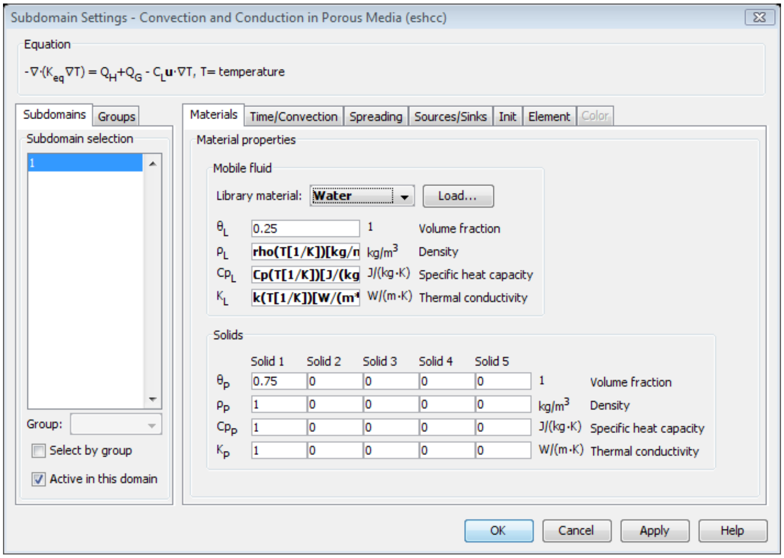
Search string:

☐ Hide undefined properties

Figure 6-8: Editing a material property.

If you want to edit the function describing some material property, click the **Functions** button. This opens the **Functions** dialog box, where you can view and edit any function describing the material.

After changing a material property in this way, you need to reload all subdomain settings that use the material; otherwise the function call does not work. To reload the material, simply go to **Physics>Subdomain Settings** and select the modified material from the **Library material** list. The new expression then shows up in the edit field for the corresponding material property in the **Subdomain Settings** dialog box (see Figure 6-9).



Subdomain Settings - Convection and Conduction in Porous Media (eshcc)

Equation

$-\nabla\cdot(K_{eq}\nabla T) = Q_H+Q_G - C_L\mathbf{u}\cdot\nabla T$, T= temperature

Subdomain selection: 1

Group:

☐ Select by group

☑ Active in this domain

Material properties

Mobile fluid

Library material: Water

θ_L	0.25	1	Volume fraction
ρ_L	rho(T[1/K])[kg/n	kg/m^3	Density
Cp_L	Cp(T[1/K])[J/(kg	J/(kg·K)	Specific heat capacity
K_L	k(T[1/K])[W/(m*	W/(m·K)	Thermal conductivity

Solids

	Solid 1	Solid 2	Solid 3	Solid 4	Solid 5		
θ_p	0.75	0	0	0	0	1	Volume fraction
ρ_p	1	0	0	0	0	kg/m^3	Density
Cp_p	1	0	0	0	0	J/(kg·K)	Specific heat capacity
K_p	1	0	0	0	0	W/(m·K)	Thermal conductivity

Figure 6-9: The update of a material property expression in the Subdomain Settings dialog box.

Note that you can only edit materials currently in the **Model** folder in this way and that any changes are local to the current model. The original material in the library file remains intact. Within the **Materials/Coefficients Library** dialog box you can, however, change a material's name and then **Copy** and **Paste** it into one of the other libraries. Afterward, clicking **OK** saves the new material for future use in the corresponding library text file.

You can also set up new materials by creating a new library file, as well as change the existing files using any text editor. A detailed description of this process appears in the *COMSOL Multiphysics User's Guide*, where you also find complete documentation on the functionality of the Materials/Coefficients Library.

7

Application Mode Reference

This chapter details the features of each application mode and its implementation in the Earth Science Module. As the subdomain equations and boundary conditions are set out in their fundamental COMSOL Multiphysics equation coefficients, review of this section is especially helpful if you want to modify the equation structure.

Overview and Organization

Application Mode Overview

The Earth Science Module provides the following application modes, organized according to the type of physics they describe:

- Fluid Flow:
  - Incompressible Navier-Stokes (2D, 3D, and 2D axi only)
  - Brinkman Equations (2D, 3D, and 2D axi only)
  - Darcy's Law: Pressure, Pressure head, and Hydraulic head analyses
  - Richards' Equation: Pressure, Pressure head, and Hydraulic head analyses
- Heat Transfer:
  - Conduction
  - Convection and Conduction
- Solute Transport:
  - Saturated Porous Media
  - Variably Saturated Porous Media

Except where otherwise is noted, the application modes are available for 1D, 2D, and 3D Cartesian geometries as well as for 1D and 2D axisymmetrical geometries.

In addition to the single-physics application modes, the Earth Science Module provides predefined couplings for modeling poroelastic media that combine the Darcy's Law application mode with COMSOL Multiphysics' application modes for structural mechanics; see the section "Poroelasticity" on page 54 for details.

Organization of the Application Mode Descriptions

The following sections detail the different features of each of the application modes offered in the Earth Science Module. For each application mode, the discussion begins by explaining how to use the dependent variables and application mode variables in expressions and postprocessing. Following are the different application mode properties you can modify (such as analysis type). After that comes a catalog of all of the information you see in the subdomain, boundary, and point settings from the **Physics** menu.

Included in this discussion is the **Equation System**. The text explains how the inputs you enter are combined in fundamental partial differential equation (PDE) forms to solve the model. Finally decision points are described and **Application Mode Variables** are defined. The application mode variables are quantities that are calculated from your inputs and the COMSOL solution. Note that you can see the definitions of the application mode variables directly in your model by going to **Physics>Equation Systems>Subdomain Settings** and choosing the **Variables** page, for example.

In describing the equation setup, a representative sample of the equations are given, so a few details and contingencies are left out. To treat the 1D, 2D, 3D, and axisymmetric cases uniformly, the space coordinates x_1, x_2, x_3 are used throughout with the following interpretations:

DIMENSION	x_1	x_2	x_3
1D	x		
2D	x	y	
3D	x	y	z
Axial symmetry, 1D	r		
Axial symmetry, 2D	r	z	

Note that you can change the default names for the space coordinates in the Model Navigator. Similarly, $u_1 = u$, $u_2 = v$, $u_3 = w$ refer to the directional components of the velocity field. Also in axisymmetric applications the line $x_1 = 0$ will be the line of symmetry.

The equation systems are provided for multiple spatial cases. The boundary conditions, however, are not shown for the axisymmetric case. The boundary conditions for axisymmetry are identical to those for Cartesian coordinates, except the flow, flux, or Neumann conditions are multiplied with the radial coordinate. The initial conditions for the dependent variables (temperature, velocity, pressure, density, turbulent kinetic energy, dissipation per unit mass, potential, and mass concentration) are not detailed because these are values that you define.

The listing of application mode and postprocessing variables, details where the information comes from as well as giving the definition. For example, a “B” indicates that the expression is available as a boundary variable. Similarly, an “S” indicates a subdomain variable, and a “V” indicates a vector plot variable.

The Incompressible Navier-Stokes Equations

This application mode is tailored for modeling free flows, typically in the absence of porous media such as in rivers, caverns, pipes, and fractures. The Navier-Stokes Equation application mode covers 2D, 3D and axisymmetry 2D. The application mode does not apply to 1D or axisymmetry in 1D because the shear terms are defined only for multiple dimension models.

The dependent variables in the Navier-Stokes Equation application mode are the fluid velocities u, v, and w in the x_1, x_2, and x_3 directions and the fluid pressure p. To use the dependent variables in equations and postprocessing, enter `u`, `v`, `w`, or `p` in an edit field or in code. Likewise `px` states the pressure gradient in the x direction, and `pt` the pressure change in time. Expressions input for coefficients and other application mode variables are designated by the suffix for the application mode name. By default the suffix is `_chns`. Therefore, to see the dynamic viscosity in equations or postprocessing, for example, enter `eta_chns` in an edit field or when coding.

For more information about the Incompressible Navier-Stokes application mode, see "The Incompressible Navier-Stokes Equations" on page 29.

Application Mode Variables

A number of variables and physical quantities are available for postprocessing and for use in equations and boundary conditions. They are listed in the Table 7-1 below.

TABLE 7-1: VARIABLES IN THE INCOMPRESSIBLE NAVIER-STOKES APPLICATION MODE

NAME	TYPE	DESCRIPTION	EXPRESSION
`rho`	S	Density	ρ
`eta`	S	Dynamic viscosity	η
F	S	Volume force	$\mathbf{F}$
U	S	Velocity field	$\lvert\mathbf{u}\rvert$
V	S	Vorticity	$\nabla \times \mathbf{u}$
K	B	Viscous force per area	$[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] \cdot \mathbf{n}$
T	B	Total force per area	$[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - p\mathbf{I}] \cdot \mathbf{n}$

TABLE 7-1: VARIABLES IN THE INCOMPRESSIBLE NAVIER-STOKES APPLICATION MODE

NAME	TYPE	DESCRIPTION	EXPRESSION
`cellRe`	S	Cell Reynolds number	$\frac{\rho\lvert\mathbf{u}\rvert h}{\eta}$
`res`	S	Equation residual	$\rho\mathbf{u}_t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \mathbf{F} - \nabla\cdot[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)]$
`res_sc`	S	Shock capturing residual	$\rho\mathbf{u}_t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \mathbf{F}$
`beta`	S	Convective field	$\rho\mathbf{u}$
`Dm`	S	Mean diffusion coefficient	η
`da`	S	Total time-scale factor	ρ
`divU`	S	Divergence of velocity field	$\nabla\cdot\mathbf{u}$
`taum`	S	GLS time scale	$\min\left(\frac{\Delta t}{\rho}, \frac{0.5h}{\max\left(\rho\lvert\mathbf{u}\rvert, \frac{6\eta}{h}\right)}\right)$
`tauc`	S	GLS time scale	$0.5\lvert\mathbf{u}\rvert h\min\left(1, \frac{\rho\lvert\mathbf{u}\rvert h}{\eta}\right)$

Note: For all variables except the dependent variables (velocities and pressure), add underscore plus the application mode name (default: chns) to the names in the list above, for example, `cellRe_chns` for the cell Reynolds number.

The Brinkman Equations

This application mode is used for modeling flow in porous media when the porosity is open enough that momentum may be dissipated through viscous shear within zones that connect free surface flows described by Navier-Stokes equations and slow subsurface flows described by Darcy's law.

The Brinkman Equation application mode is available in 2D, 3D as well as axisymmetry 2D. The application mode does not apply to 1D or axisymmetry in 1D because the shear terms are defined only for multiple dimension models. Like the Navier-Stokes equations, the dependent variables in the Brinkman Equation application mode are the fluid velocities u, v, and w in the x_1, x_2, and x_3 directions and the fluid pressure p. To use the dependent variables in equations and postprocessing, enter `u`, `v`, `w`, or `p` in an edit field or in code. Likewise `px` states the pressure gradient in the x direction, and `pt` the pressure change in time. Expressions input for coefficients and other application mode variables are designated by the suffix for the application mode name. By default the suffix is `_chbr`. Therefore, to see the dynamic viscosity in equations or postprocessing, for example, type `eta_chbr` in a dialog box or when coding.

For more information about the Brinkman Equation application mode, see "The Brinkman Equations" on page 27.

Application Mode Variables

The variables and physical quantities available for postprocessing and for use in equations and boundary conditions are the same as for the Incompressible Navier-Stokes application mode; see Table 7-1 on page 106.

Darcy's Law

This application mode describes fluid flow in porous media driven by gradients in pressure and gravitational potential. The dependent variable in Darcy's law always is pressure p but interfaces for inputs in hydraulic head H and pressure head H_p are provided. To use the dependent variable in equations and postprocessing you enter `p` in an edit field or in code. Likewise `px` states the pressure gradient in the x direction, and `pt` the pressure change in time. As H and H_p results from calculations they are application mode variables designated by the suffix for the application mode name. By default the suffix for Darcy's law is `_esdl`. To use H and H_p in equations or postprocessing, enter `H_esdl` or `Hp_esdl` in an edit field or when coding. You can also invoke the suffix to use other application mode variables in expressions. With the saturated hydraulic conductivity K_s, for instance, enter `Ks_esdl` in your expression.

PDE Formulation

The governing equation for fluid flow described by Darcy's law is:

$$\delta_S S\frac{\partial p}{\partial t} + \nabla\cdot\left[-\delta_K\frac{\kappa}{\eta}(\nabla p + \rho_f g\nabla D)\right] = \delta_Q Q_s$$

where S is the storage coefficient, κ is permeability, η is dynamic viscosity; ρ_f is the fluid density; g is acceleration of gravity; D is the vertical elevation; and Q_s is the volumetric flow rate per unit volume of porous medium for a fluid source. The terms g and D are variables that you define in the **Application Scalar Variables** dialog box. These terms can be defined with numbers or expressions, including those that involve results from other equations in your model. Also added to the equation are optional scaling coefficients δ for each major term S, K, and Q. The scaling coefficients are helpful for modeling density variations and mobile and immobile domain flows, for example.

If hydraulic conductivity K is used to describe the transmissive properties in lieu of permeability, the equations takes the form:

$$\delta_S S\frac{\partial p}{\partial t} + \nabla\cdot\left[-\delta_K\frac{K}{\rho_f g}(\nabla p + \rho_f g\nabla D)\right] = \delta_Q Q_s$$

In the equations κ and K are tensors defined as $\kappa = A_r\kappa_s$ and $K = A_r K_s$. Where and κ_s and K_s denote the value of intrinsic permeability and saturated hydraulic conductivity, respectively, and A_r is a tensor of anisotropy ratios. Also appearing in the equation are optional scaling coefficients for each major term S, K, and Q.

Analysis Types

The **Variable** application mode property denote the interfaces for p, H and $H_{p.}$ You can choose which analysis type directly from the **Model Navigator** as you would a different application mode. The predefined option for storage coefficient S_s depends on the analysis type (see "Coefficients" below).

When the analysis type is p

$$S_s = [\chi_p(1-\theta_s) + \chi_p\theta_s]$$

The definition for H reads

$$H = \frac{p}{\rho_f g} + D \qquad S_s = \frac{[\chi_p(1-\theta_s) + \chi_p\theta_s]}{\rho_f g}$$

For H_p the definition is

$$H_p = \frac{p}{\rho_f g} \qquad S_s = \frac{[\chi_p(1-\theta_s) + \chi_p\theta_s]}{\rho_f g}$$

Subdomain Settings

The **Subdomain Settings** dialog box contains the following pages:

- **Coefficients**
- **Scaling Factors**
- **Init**
- **Element**

COEFFICIENTS

The **Coefficients** page contains edit fields to input porous media properties for your model.

SYMBOL	VARIABLE	DESCRIPTION	OPTIONS
S	S	Storage coefficient	(1) Specific storage (2) User defined
θ_s	`thetas`	Volume liquid fraction	

SYMBOL	VARIABLE	DESCRIPTION	OPTIONS
χ_f	`chif`	Compressibility of fluid	
χ_p	`chip`	Compressibility of solid	
K_s	`Ks`	Saturated hydraulic conductivity	
κ_s	`kaps`	Permeability	
A_r	`Ar`	Tensor of anisotropy ratios	
ρ_f	`rhof`	Fluid density	
η	`eta`	Dynamic viscosity	
Q_s	`Qs`	Fluid source	
α_b	`alpha_b`	Biot-Willis coefficient	

Note: The Biot-Willis coefficient is available only when using the Poroelasticity predefined multiphysics coupling.

SCALING FACTORS

The **Scaling Factors** page provides optional coefficients that you can use to scale different terms in your model. The scaling factors are helpful for modeling density variations and immobile and mobile domains, for example.

SYMBOL	VARIABLE	DESCRIPTION
d_S	`CSs`	Scaling coefficient, Storage
d_K	`CKs`	Scaling coefficient, Flux
d_Q	`CQs`	Scaling coefficient, Source

Boundary Settings

The boundary conditions are as follows.

TYPE	BOUNDARY CONDITION—P	DESCRIPTION
H0	$p = p_0$	Pressure
Hw	$p = 0$	Water table/Seepage face
N0	$-\mathbf{n} \cdot \left[-\frac{\underline{\underline{\kappa}}}{\eta}\nabla(p + \rho_f g D)\right] = N_0$	Inward flux

TYPE	BOUNDARY CONDITION—P	DESCRIPTION
Nz	$\mathbf{n}\cdot\left[\frac{\underline{\kappa}}{\eta}\nabla(p+\rho_{\mathrm{f}}gD)\right] = 0$	Zero flux/Symmetry
Nm	$-\mathbf{n}\cdot\left[-\frac{\underline{\kappa}}{\eta}\nabla(p+\rho_{\mathrm{f}}gD)\right]$ $= N_0+R_{\mathrm{b}}[(p_{\mathrm{b}}-p)+\rho_{\mathrm{f}}g(D_b-D)]$	Mixed
Na	$\mathbf{n}\cdot\left[-\frac{\underline{\kappa}}{\eta}\nabla(p+\rho_{\mathrm{f}}gD)\right] = 0$	Axial symmetry

When posed for hydraulic head and pressure head the following equations appear:

TYPE	BOUNDARY CONDITION—H	BOUNDARY CONDITION—HP	DESCRIPTION
H0	$H=H_0$	$H_p=H_{p0}$	Hydraulic head Pressure head
Hw	$H=D$	$H_p=0$	Water table/Seepage face
N0	$-\mathbf{n}\cdot(-K\nabla H) = N_0$	$-\mathbf{n}\cdot[-K\nabla(H_p+D)] = N_0$	Inward flux
Nz	$\mathbf{n}\cdot(K\nabla H) = 0$	$\mathbf{n}\cdot[K\nabla(H_p+D)] = 0$	Zero flux/Symmetry
Nm	$-\mathbf{n}\cdot(-K\nabla H)$ $= N_0+R_{\mathrm{b}}(H_{\mathrm{b}}-H)$	$-\mathbf{n}\cdot[-\underline{K}\nabla(H_p+D)]$ $= N_0+R_{\mathrm{b}}[(H_{p\mathrm{b}}-H_p)+(D_b-D)]$	Mixed
Na	$\mathbf{n}\cdot(-K\nabla H) = 0$	$\mathbf{n}\cdot[-K\nabla(H_p+D)] = 0$	Axial symmetry

Point and Edge Settings

Point Settings (2D and 3D) and Edge Settings (3D) are given in the following table. Options for both stationary and time-dependent inputs are available. In time-dependent simulations, the point may switch from a specified p, H, or H_p to a specified flux. If both p, H, or H_p and a flux are specified on the same point or edge for the same time, the specified pressure will be simulated, and the specified flux will be neglected.

SYMBOL	VARIABLE	ANALYSIS	DESCRIPTION
p_0	p0	stationary	Pressure
p_0	p0	transient	Pressure
t_{p0}	`tp0`	transient	Starting time, Pressure

SYMBOL	VARIABLE	ANALYSIS	DESCRIPTION
t_{pf}	`tpf`	transient	Ending time, Pressure
q_0	`q0`	stationary	Flux
q_0	`q0`	transient	Flux
t_{q0}	`tq0`	transient	Starting time, flux
t_{qf}	`tqf`	transient	Ending time, flux

Scalar Variables

A scalar variable δ_{ts} defines the time scale over which step changes in specified pressures and fluxes are smoothed with a Heaviside function. It is defined by the same value or expression throughout the model. Likewise, the acceleration of gravity g and the direction in which gravity acts D are defined as numbers, expressions, or as results from other equations in the **Application Scalar Variables** dialog box for the entire geometry and simulation period. Being able to arbitrarily define D and g allows for modeling flows in different gravitational settings, Mars for instance. The time scaling term facilitates modeling step function constraints on points and edges. For more information see the section “Point and Edge Settings” above.

SYMBOL	VARIABLE	DESCRIPTION
D	`D`	Elevation/vertical axis
g	`g`	Gravity
t_s	`tscale`	Heaviside scaling factor

Application Mode Variables

Table 7-2 lists the application mode variables in the Darcy’s Law application mode. These variables are available for use in terms and expressions. When accessing them, append an underscore followed by the suffix for the application mode name.

In the Analysis column, p stands for Pressure analysis, H for Hydraulic head analysis, and Hp for Pressure head analysis.

TABLE 7-2: VARIABLES IN THE DARCY’S LAW APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
`CSs`	All	B/S/E/P	Scaling coefficient, Storage	δ_{Ss}
`CKs`	All	B/S/E/P	Scaling coefficient, Cond/Perm	δ_{Ks}
`CQs`	All	B/S/E/P	Scaling coefficient, Source	δ_{Qs}

TABLE 7-2: VARIABLES IN THE DARCY'S LAW APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
`S`	H, Hp	B/S/E/P	Storage term	$\frac{(\chi_p(1-\theta_s)+\chi_f\theta_s)\delta_{Ss}}{\rho_f g}$ (specific storage) $\frac{S\delta_{Ss}}{\rho_f g}$ (user defined)
`S`	p	B/S/E/P	Storage term	$(\chi_p(1-\theta_s)+\chi_f\theta_s)\delta_{Ss}$ (specific storage) $S\delta_{Ss}$ (user defined)
`Qs`	All	B/S	Fluid sources	$Q_s\delta_{Qs}$
`K`	All	B/S/E/P	Hydraulic conductivity tensor	$K_s\delta K_s$
`Kxixj`	All	B/S/E/P	Hydraulic conductivity tensor, x_ix_j component	K_{ij}
`kap`	All	B/S/E/P	Permeability tensor	$\kappa_s\delta_{Ks}$
`kapxixj`	All	B/S/E/P	Permeability tensor, x_ix_j component	κ_{sij}
`rhof`	All	B/S/E/P	Fluid density	ρ_f
`g`	All	B/S/E/P	Gravity	g
`D`	All	B/S/E/P	Vertical coordinate	D
`p`	All	B/S/E/P	Pressure	p
`gradp`	All	B/S/E/P	Pressure gradient, norm	$\|\nabla p\|$
`pxi`	All	V	Pressure gradient, x_i component	$\frac{\partial p}{\partial x_i}$
`Hp`	Hp	B/S/E/P	Pressure head	$p/(\rho_f g)$
`gradHp`	Hp	B/S/E/P	Pressure head gradient, norm	$\|\nabla H_p\|$
`Hpxi`	Hp	V	Pressure head gradient, x_i component	$\frac{\partial H_p}{\partial x_i}$
`H`	H	B/S/E/P	Hydraulic head	$p/(\rho_f g)+D$
`gradH`	H	B/S/E/P	Hydraulic head gradient, norm	$\|\nabla(H)\|$
`Hxi`	H	V	Hydraulic head gradient, x_i component	$\frac{\partial H}{\partial x_i}$

TABLE 7-2: VARIABLES IN THE DARCY'S LAW APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
`u`, `v`, `w`	All	V	Darcy velocity x_i	$-\frac{\kappa}{\eta}\frac{\partial}{\partial x_i}(p+\rho_f g D)$ (permeability) $-\frac{K}{\rho_f g}\frac{\partial}{\partial x_i}(p+\rho_f g D)$ (conductivity)
`U`	All	B/S/E/P	Total Darcy velocity	$\sqrt{u^2+v^2+w^2}$
`nU`	All	B	Normal Darcy velocity	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_f g D)\right]$ (permeability) $-\mathbf{n}\cdot\left[-\frac{K}{\rho_f g}\nabla(p+\rho_f g D)\right]$ (conductivity)
`flux`	All	B	Boundary flux	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_f g D)\right]$ (permeability) $-\mathbf{n}\cdot\left[-\frac{K}{\rho_f g}\nabla(p+\rho_f g D)\right]$ (conductivity)

Note: Append an underscore plus the application mode name (default: esdl) to the application mode names in the list above, except for the dependent variable (pressure). For example, `flux_esdl` is the variable for the boundary flux.

Richards' Equation

This application mode describes fluid flow in variably saturated porous media. The flow is driven by gradients in pressure and gravitational potential. Application modes are available for 1D, 2D, 3D, axisymmetry in 1D, and axisymmetry in 2D.

As with Darcy's law, the dependent variable always is pressure p. Interfaces for inputs in hydraulic head H and pressure head H_p are provided. To use the dependent variable in equations and postprocessing, enter `p` in an edit field or in code. Likewise `px` states the pressure gradient in the x direction, and `pt` the pressure change in time. As H and H_p results from calculations they are application mode variables designated by the suffix for the application mode name. By default the suffix for the Richards' Equation application mode is `_esvr`. To use H and H_p in equations or postprocessing, enter `H_esvr` or `Hp_esvr` in an edit field or when coding. You can also invoke the suffix to use other application mode variables in expressions. With the saturated hydraulic conductivity K_s, for instance, enter `Ks_esvr` in your expression.

PDE Formulation

Richards' equation is

$$\delta_{\mathrm{ts}}[C + \mathrm{Se}S]\frac{\partial p}{\partial t} + \nabla \cdot \left[-\frac{\kappa}{\eta}k_{\mathrm{r}}\nabla(p + \rho_{\mathrm{f}}gD)\right] = Q_{\mathrm{s}}$$

where C is the specific moisture capacity, Se is the effective saturation, S is the storage coefficient, κ is the permeability tensor, η is dynamic viscosity, k_{r} is the relative permeability, ρ_{f} is the fluid density, g is the acceleration of gravity, D is the vertical elevation, and Q_{s} is the volumetric flow rate per unit volume of porous medium for a fluid source. You can set the values of the variables g and D in the **Application Scalar Variables** dialog box that appears when choosing **Physics>Scalar Variables**. They can be defined as numbers or expressions, including those that involve results from other equations in your model. The scaling coefficient, δ_{ts}, is optional.

The equation can also be solved in terms of hydraulic conductivity by substituting the following:

$$\frac{\kappa}{\eta} = A_{\mathrm{r}}\frac{K_{\mathrm{s}}}{\rho_{\mathrm{f}}g} = A_{\mathrm{r}}\frac{\kappa_{\mathrm{s}}k_{\mathrm{r}}}{\eta}$$

In this equation, κ_s and K_s are the intrinsic permeability and the saturated hydraulic conductivity, respectively, and A_r is a tensor of anisotropy ratios.

The volume fraction of the fluid, θ, varies with H_p.

$$H_p = H - D = \frac{p}{\rho_f g_r}$$

The equation coefficients C, Se, and k_r vary with θ and H_p for unsaturated conditions and become constant when the system reaches saturation:

$$\begin{array}{lllll}\theta = \theta(H_p), & C = C(\theta, H_p), & \mathrm{Se} = \mathrm{Se}(\theta, H_p), & k_r = k_r(\theta, H_p), & \text{if unsaturated} \\ \theta = \theta_s, & C = 0, & \mathrm{Se} = 1, & k_r = 1, & \text{if saturated}\end{array}$$

Whether the system is unsaturated or saturated depends on H_p. The section "Subdomain Settings" below gives the details of different methods for describing θ, C, Se, and k_r, as well as how the dividing line between saturated and unsaturated conditions is defined.

Analysis Types

The **Variable** application mode property denotes the interfaces for p, H, and H_p. You can choose analysis type directly from the **Model Navigator**, as you would choose a different application mode. How C is used in the equation and the predefined option for storage coefficient S_s depends on the analysis type (see "Coefficients" below).

When the analysis type is p, these quantities are defined as

$$S_s = [\chi_p(1-\theta_s) + \chi_p\theta_s], \qquad C = \frac{C(H_p)}{\rho_f g}$$

The definitions for analysis type H read

$$H = \frac{p}{\rho_f g} + D \qquad S_s = \frac{[\chi_p(1-\theta_s) + \chi_p\theta_s]}{\rho_f g} \qquad C = C(H_p)$$

For H_p the definitions are

$$H_p = \frac{p}{\rho_f g} \qquad S_s = \frac{[\chi_p(1-\theta_s) + \chi_p\theta_s]}{\rho_f g} \qquad C = C(H_p)$$

Subdomain Settings

The following tables give the parameters and equation coefficients for subdomain settings dialogs. Included are the following pages:

- **Coefficients**
- **van Genuchten**
- **Brooks & Corey**
- **User Defined**
- **Init**
- **Element**

COEFFICIENTS

The **Coefficients** page provides expression fields for:

SYMBOL	VARIABLE	DESCRIPTION	OPTIONS
	`constReltype`	Permeability and retention	(1) Van Genuchten (2) Brooks & Corey (3) User defined
S	`S`	Storage coefficient	(1) Specific storage (2) User defined
θ_s	`thetas`	Volume liquid fraction, saturation	
θ_r	`thetar`	Volume liquid fraction, residual	
χ_f	`chif`	Compressibility of fluid	
χ_p	`chip`	Compressibility of solid	
K_s	`Ks`	Saturated hydraulic conductivity	
κ_s	`kaps`	Intrinsic permeability	
A_r	`Ar`	Tensor of anisotropy ratios	
ρ_f	`rhof`	Fluid density	
η	`eta`	Dynamic viscosity	
Q_s	`Qs`	Fluid source	

VAN GENUCHTEN AND BROOKS & COREY

The **van Genuchten** and **Brooks & Corey** pages provide expression fields for:

COEFFICIENT	VARIABLE VAN GENUCHTEN	VARIABLE BROOKS & COREY	DESCRIPTION
α	`alpha_vG`	`alpha_BC`	alpha constant
n	`n_vG`	`n_BC`	n constant
l	`l_vG`	`l_BC`	l constant

When the **van Genuchten** page is active the retention and permeability relationships are defined according to:

$$\theta = \begin{cases} \theta_\mathrm{r} + \mathrm{Se}(\theta_\mathrm{s} - \theta_\mathrm{r}) & H_p < 0 \\ \theta_\mathrm{s} & H_p \ge 0 \end{cases}$$

$$\mathrm{Se} = \begin{cases} \dfrac{1}{[1 + |\alpha H_p|^n]^m} & H_p < 0 \\ 1 & H_p \ge 0 \end{cases}$$

$$C = \begin{cases} \dfrac{\alpha m}{1-m}(\theta_\mathrm{s} - \theta_\mathrm{r})\mathrm{Se}^{\frac{1}{m}}\left(1 - \mathrm{Se}^{\frac{1}{m}}\right)^m & H_p < 0 \\ 0 & H_p \ge 0 \end{cases} \cdot$$

$$k_\mathrm{r} = \begin{cases} \mathrm{Se}^l\left[1 - \left(1 - \mathrm{Se}^{\frac{1}{m}}\right)^m\right]^2 & H_p < 0 \\ 1 & H_p \ge 0 \end{cases}$$

$$m = 1 - \frac{1}{n}$$

These relations, as defined by **Brooks & Corey** are:

$$\theta = \begin{cases} \theta_r + \mathrm{Se}(\theta_s - \theta_r) & H_p < -\dfrac{1}{\alpha} \\ \theta_s & -\dfrac{1}{\alpha} \le H_p \end{cases}$$

$$\mathrm{Se} = \begin{cases} \dfrac{1}{|\alpha H_p|^n} & H_p < -\dfrac{1}{\alpha} \\ 1 & -\dfrac{1}{\alpha} \le H_p \end{cases}$$

$$C = \begin{cases} \dfrac{-n}{H_p}(\theta_s - \theta_r)\dfrac{1}{|\alpha H_p|^n} & H_p < -\dfrac{1}{\alpha} \\ 0 & -\dfrac{1}{\alpha} \le H_p \end{cases}$$

$$k_r = \begin{cases} \mathrm{Se}^{\frac{2}{n} + l + 2} & H_p < -\dfrac{1}{\alpha} \\ 1 & -\dfrac{1}{\alpha} \le H_p \end{cases}$$

USER DEFINED

With the **User defined** option, you fill the expression fields with functions for θ, C, Se, and k_r. These functions can be interpolations defined in the **Functions** dialog box, which appears when you select **Options>Functions**. You also define the value of the pressure head, H_p, below which these functions are active. This definition can be posed such that it accounts for pressure/saturation relationships of multiple phases.

COEFFICIENT	USER DEFINED	APPLICATION MODE VARIABLE DEFINITION
α_i	`alpha_i`	Pressure head (Hp) at onset of saturation
θ	`theta_i`	Liquid volume faction (Hp < α)
C	`C_i`	Specific moisture capacity (Hp < α)
Se	`Se_i`	Effective saturation (Hp < α)
k_r	`kr_i`	Relative permeability function (Hp < α)

Boundary Settings

The boundary conditions for pressure are:

TYPE	BOUNDARY CONDITION—P	DESCRIPTION
H0	$p = p_0$	Pressure
Hw	$p = 0$	Atmosphere or gauge
N0	$-\mathbf{n} \cdot \left[-\frac{\kappa}{\eta} k_\mathrm{r} \nabla(p + \rho_\mathrm{f} g D)\right] = N_0$	Inward flux
Nz	$\mathbf{n} \cdot \left[\frac{\kappa}{\eta} k_\mathrm{r} \nabla(p + \rho_\mathrm{f} g D)\right] = 0$	Zero flux/Symmetry
Nm	$-\mathbf{n} \cdot \left[-\frac{\kappa}{\eta} k_\mathrm{r} \nabla(p + \rho_\mathrm{f} g D)\right]$ $= N_0 + R_\mathrm{b}[(p_\mathrm{b} - p) + \rho_\mathrm{f} g (D_\mathrm{b} - D)]$	Mixed
Na	$\mathbf{n} \cdot \left[-\frac{\kappa}{\eta} k_\mathrm{r} \nabla(p + \rho_\mathrm{f} g D)\right] = 0$	Axial symmetry

The following interfaces pose the above boundaries in terms of hydraulic head and pressure head.

TYPE	BOUNDARY CONDITION—H	BOUNDARY CONDITION—HP	DESCRIPTION
H0	$H = H_0$	$H_p = H_{p0}$	Hydraulic head Pressure head
Hw	$H = D$	$H_p = 0$	Atmosphere or gauge
N0	$-\mathbf{n} \cdot (-K k_\mathrm{r} \nabla H) = N_0$	$-\mathbf{n} \cdot [-K k_\mathrm{r} \nabla(H_p + D)] = N_0$	Inward flux
Nz	$\mathbf{n} \cdot (K k_\mathrm{r} \nabla H) = 0$	$\mathbf{n} \cdot [K k_\mathrm{r} \nabla(H_p + D)] = 0$	Zero flux/Symmetry
Nm	$-\mathbf{n} \cdot (-K k_\mathrm{r} \nabla H)$ $= N_0 + R_b(H_b - H)$	$-\mathbf{n} \cdot [-K k_\mathrm{r} \nabla(H_p + D)]$ $= N_0 + R_\mathrm{b}[(H_{p\mathrm{b}} - H_p) + (D_b - D)]$	Mixed
Na	$\mathbf{n} \cdot (-K k_\mathrm{r} \nabla H) = 0$	$\mathbf{n} \cdot [-K k_\mathrm{r} \nabla(H_p + D)] = 0$	Axial symmetry

Point Settings, Edge Settings, and Scalar Variables

The Point Settings (2D, 2D-axisymmetric, 3D), Edge Settings (3D), and Scalar Variables for the Richards' Equation application mode are identical to those described for Darcy's Law; see page 112 and page 113 in the section "Darcy's Law" on page 109.

Application Mode Variables

Table 7-3 lists the application mode variables in the Richard's Equation application mode. In the Analysis column p stands for Pressure analysis, H for Hydraulic head analysis, and Hp for Pressure head analysis.

TABLE 7-3: VARIABLES IN THE RICHARD'S EQUATION APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
`Cts`	All	S/B/E/P	Time scaling coefficient	δ_{ts}
`C`	All	S/B/E/P	Specific moisture capacity	$\frac{C_{\mathrm{vG}}}{\rho_{\mathrm{f}} g}$ (van Genuchten) $\frac{C_{\mathrm{BC}}}{\rho_{\mathrm{f}} g}$ (Brooks and Corey) $\frac{C_i}{\rho_{\mathrm{head}} g}$ (user defined)
`Se`	All	S/B/E/P		$\mathrm{Se}_{\mathrm{vG}}$ (van Genuchten) $\mathrm{Se}_{\mathrm{BC}}$ (Brooks and Corey) Se_i (user defined)
`S`	p	S/B/E/P	Storage term	$\chi_p(1-\theta_{\mathrm{s}})+\chi_{\mathrm{f}}\theta_{\mathrm{s}}$ (specific storage) S_i (user defined)
`S`	Hp	S/B/E/P	Storage term	$\chi_p(1-\theta_{\mathrm{s}})+\chi_{\mathrm{f}}\theta_{\mathrm{s}}$ (specific storage) $\frac{S_i}{\rho_{\mathrm{f}} g}$ (user defined)
`p`	p	S/B/E/P	Pressure	p
`kaponeta`	p	S/B/E/P	Permeability on viscosity	$\frac{\kappa}{\eta}=\frac{K}{\rho_{\mathrm{f}} g_{\mathrm{r}}}$
`K`	All	S/B/E/P	Hydraulic conductivity tensor	$K_{\mathrm{s}}\kappa_{\mathrm{r}}$
`kap`	All	S/B/E/P	Permeability tensor	$\kappa_{\mathrm{s}}k_{\mathrm{r}}$
`rhof`	All	S/B/E/P	Fluid density	ρ_{f}
`g`	All	S/B/E/P	Gravity	g
`eta`	All	S/B/E/P	Fluid viscosity	η
`D`	All	S/B/E/P	Vertical coordinate	D

TABLE 7-3: VARIABLES IN THE RICHARD'S EQUATION APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
`Qs`	All	S/B/E/P	Fluid sources	Q_s
`Hp`	p	S/B/E/P	Pressure head	$\frac{p}{\rho_f g_r}$
`Hp`	Hp	S/B/E/P	Pressure head	H_p
`Hp`	H	S/B/E/P	Pressure head	$H - D$
`m`	All	S/B/E/P	m constant	$1 - \frac{1}{n}$
`theta`	All	S/B/E/P	Liquid volume fraction	$\begin{array}{ll} (\theta_r + (\theta_s - \theta_r)\mathrm{Se}) & (H_p < 0) \\ \theta_s & (H_p \ge 0) \end{array}$ (van Genuchten) $\begin{array}{ll} (\theta_r + (\theta_s - \theta_r)\mathrm{Se}) & \left(H_p < -\frac{1}{\alpha}\right) \\ \theta_s & \left(H_p \ge -\frac{1}{\alpha}\right) \end{array}$ (Brooks and Corey) $\begin{array}{l} \theta_i \ (H_p < \alpha) \\ \theta_s \ (H_p \ge \alpha) \end{array}$ (user defined)

TABLE 7-3: VARIABLES IN THE RICHARD'S EQUATION APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
C	All	S/B/E/P	Specific moisture capacity	$\frac{\alpha m}{1-m}(\theta_\mathrm{s}-\theta_\mathrm{r})\mathrm{Se}^{\frac{1}{m}}\left(1-\mathrm{Se}^{\frac{1}{m}}\right)^{m}$ $(H_p<0)$ 0 $(H_p\geq 0)$ (van Genuchten) $-\frac{n}{H_p}(\theta_\mathrm{s}-\theta_\mathrm{r})(\alpha H_p)^{-n}$ $\left(H_p<-\frac{1}{\alpha}\right)$ 0 $\left(H_p\geq-\frac{1}{\alpha}\right)$ (Brooks and Corey) C_i $(H_p<\alpha)$ 0 $(H_p\geq\alpha)$ (user defined)
Se	All	S/B/E/P	Effective saturation	$(1+(\alpha H_p)^{n})^{-m}$ $(H_p<0)$ 1 $(H_p\geq 0)$ (van Genuchten) αH_p^{-n} $\left(H_p<-\frac{1}{\alpha}\right)$ 1 $\left(H_p\geq-\frac{1}{\alpha}\right)$ (Brooks and Corey) Se_i $(H_p<\alpha)$ 1 $(H_p\geq\alpha)$ (user defined)

TABLE 7-3: VARIABLES IN THE RICHARD'S EQUATION APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
`kr`	All	S/B/E/P	Relative permeability	$\mathrm{Se}^{l}\left(1-\left(1-\mathrm{Se}^{\frac{1}{m}}\right)^{m}\right)^{2} \quad (H_p < 0)$ $1 \quad (H_p \geq 0)$ (van Genuchten) $\mathrm{Se}^{\frac{2}{n}+l+2} \quad \left(H_p < -\frac{1}{\alpha}\right)$ $1 \quad \left(H_p \geq -\frac{1}{\alpha}\right)$ (Brooks and Corey) $k_{\mathrm{r}i} \ (H_p < \alpha)$ $1 \ (H_p \geq \alpha)$ (user defined)
`gradp`	All	B/S/E/P	Pressure gradient, norm	$\lvert\nabla p\rvert$
`p`*`xi`*	All	V	Pressure gradient, x_i component	$\frac{\partial p}{\partial x_i}$
`gradHp`	Hp	B/S/E/P	Pressure head gradient, norm	$\lvert\nabla H_p\rvert$
`Hp`*`xi`*	Hp	V	Pressure head gradient, x_i component	$\frac{\partial H_p}{\partial x_i}$
`gradH`	H	B/S/E/P	Hydraulic head gradient, norm	$\lvert\nabla(H)\rvert$
`H`*`xi`*	H	V	Hydraulic head gradient, x_i component	$\frac{\partial H}{\partial x_i}$
`u`, `v`, `w`	p	S/B/E/P	Darcy velocity, x_i component	$-\frac{\kappa}{\eta}\frac{\partial}{\partial x_i}(p+\rho_{\mathrm{f}} g_{\mathrm{r}} D)$
`U`	All	S/B/E/P	Total Darcy velocity	$\sqrt{u^2+v^2+w^2}$

TABLE 7-3: VARIABLES IN THE RICHARD'S EQUATION APPLICATION MODE

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
`nU`	all	B/E/P	Normal Darcy velocity	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_f g_r D)\right]$
`flux`	all	B/E/P	Boundary flux	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_f g_r D)\right]$

Note: Append an underscore plus the application mode name (default: `esvr`) to the application mode names in the list above, except for the dependent variable (pressure). For example, `flux_esvr` is the variable for the boundary flux.

Conduction

This application mode is used for modeling heat transport by conduction in media with multiple constituents (for example, porous media) and those made up of one component (for example, solids). The dependent variable is temperature T. To use the dependent variable in equations and postprocessing, enter `T` in an edit field or in code. Likewise `Tx` states the temperature gradient in the x direction, and `Tt` the temperature change in time. Expressions input for coefficients and other application mode variables are designated by the suffix for the application mode name. By default the suffix is `_eshc`. Therefore, to see the equivalent heat capacity in equations or postprocessing, enter `Keq_eshc` in an edit field or when coding.

PDE Formulation

The equation governing heat transfer by conduction is:

$$\delta_{\mathrm{ts}}\ C_{\mathrm{eq}}\frac{\partial T}{\partial t}+\nabla\cdot(-K_{\mathrm{eq}}\nabla T)\ \ =Q_H+Q_G+Q_C+Q_R$$

where Q_H, Q_G, Q_C, and Q_R, respectively, are distributed sources of heat for general, geothermal, convective, and radiative cases. Q_C and Q_R are available for 1D and 2D geometries to facilitate modeling transversal heat transfer on boundaries.

Application Mode Properties

The **Application Mode Properties** dialog box available in the **Physics** menu or from the **Model Navigator** allow the choice of materials in the model. The **Porous Media** option triggers a table that allows inputs for up to five fluids and solids. With the **Solid** option, the table provides inputs for up to five solids.

Subdomain Settings

The **Subdomain Settings** dialog boxes contain interfaces for five categories of options: (1) **Materials**, (2) **Thermal Properties**, (3) **Sources/Sinks**, (4) **Init**, and (5) **Element**.

MATERIALS

The **Materials** page is an optional dialog for you to input properties of materials in the model. Spaces are available for up to five fluids and five solids. In this application mode, the fluids are assumed immobile. The interface provides edit fields for the following properties:

TERM	VARIABLE	DESCRIPTION
θ_L	`thetaL`	Volume fraction, liquid
ρ_L	`rhoL`	Density, liquid
C_{pL}	`CpL`	Specific heat capacity, liquid
K_L	`KL`	Thermal conductivity, liquid
θ_P	`thetaP`	Volume fraction, solid
ρ_P	`rhoP`	Density, solid
C_{pP}	`CpP`	Specific heat capacity, solid
K_P	`KP`	Thermal conductivity, solid

You can choose to automatically calculate any or all of the following as volume averages based on the information in the table: C_{eq}, K_{eq}, and ρ_{geo}.

THERMAL PROPERTIES

On the **Thermal Properties** page you enter various equation coefficients and choose how to calculate effective properties.

TERM	VARIABLE	DESCRIPTION	OPTIONS
δ_{ts}	`Dts`	Scaling coefficient, time	
C_{eq}	`Ceq`	Equivalent volume heat capacity	(1) calculated volume average (2) user defined
K_{eq}	`Keq`	Equivalent thermal conductivity	(1) calculated volume average (2) user defined
A_{r}	`Ar`	Anisotropy ratios	

SOURCES/SINKS

The **Sources/Sinks** page prompts for information needed to define the source terms Q_H, Q_G, Q_C, and Q_R as follows:

TERM	VARIABLE	DESCRIPTION	OPTIONS
Q_H	`QH`	General heat source	
Q_G	`QG`	Geothermal heat production	(1) uniform (2) exponential (3) user defined

TERM	VARIABLE	DESCRIPTION	OPTIONS
ρ_{geo}	`rhogeo`	Geothermal density	(1) calculated, solid (2) calculated, porous media (3) user defined
q_{geo}	`qgeo`	Radiogenic heating per mass	
z_{geo}	`zgeo`	Depth	
h_{geo}	`hgeo`	Length scale	

Boundary Settings

The following table sets out the boundary conditions for heat transfer analysis with conduction:

TYPE	BOUNDARY CONDITION	DESCRIPTION
T	$T = T_0$	Temperature
T0	$T = 0$	Zero temperature
N0	$\mathbf{n} \cdot (K_{\mathrm{eq}} \nabla T) = N_0 + h(T_{\mathrm{inf}} - T) + C_{\mathrm{const}}({T_{\mathrm{amb}}}^4 - T^4)$	Heat flux
Nz	$\mathbf{n} \cdot (K_{\mathrm{eq}} \nabla T) = 0$	Insulation/Symmetry
ax	$\mathbf{n} \cdot (K_{\mathrm{eq}} \nabla T) = 0$	Axial symmetry

Point Settings and Edge Settings

Point Settings (2D and 3D) and Edge Settings (3D) are given in the following table. Options for both stationary and time-dependent inputs are available. In time-dependent simulations, the point may switch from a specified temperature to a specified flux. If both a temperature and a flux are specified on the same point or edge for the same time, the specified temperature will be simulated, and the specified flux will be neglected.

SYMBOL	VARIABLE	ANALYSIS	DESCRIPTION
T_0	`T0`	stationary	Temperature
T_0	`T0`	transient	Temperature
t_{T0}	`tT0`	transient	Starting time, temperature
$t_{T\mathrm{f}}$	`tTf`	transient	Ending time, temperature

SYMBOL	VARIABLE	ANALYSIS	DESCRIPTION
N_0	`N0`	stationary	Flux
N_0	`N0`	transient	Flux
t_{N0}	`tN0`	transient	Starting time, flux
$t_{N\mathrm{f}}$	`tNf`	transient	Ending time, flux

Scalar Variables

The time scale over which step changes in specified temperatures and fluxes are smoothed with a Heaviside function is defined by a scalar variable so that it is defined on the same value or expression throughout the model.

SYMBOL	VARIABLE	DEFAULT	DESCRIPTION
t_s	`tscale`	`1e-5`	Heaviside scaling factor

Application Mode Variables

Table 7-4 lists the application mode variables for the Conduction application mode. These variables are available in equations and for postprocessing. For some of them, the definition depends on the analysis type or user-defined options. In the Analysis column, S stands for Solid and PM for Porous Media.

TABLE 7-4: VARIABLES IN THE CONDUCTION APPLICATION MODE

ANALYSIS	NAME	TYPE	DESCRIPTION	EXPRESSION
S, PM	`Dts`	S	Time scaling coefficient	δ_ts
S	`Ceq`	S	Volume heat capacity (equiv)	$\Sigma(\theta_{Pi}C_{Pi})/\Sigma\theta_{Pi}$
PM	`Ceq`	S	Volume heat capacity (equiv)	$[\Sigma(\theta_{Pi}C_{Pi})+\Sigma(\theta_{Li}C_{Li})]/$ $[\Sigma\theta_{Pi}+\Sigma\theta_{Li}]$
S	`Keq`	S	Thermal conductivity (equiv)	$\Sigma(\theta_{Pi}K_{Pi})/\Sigma\theta_{Pi}$
PM	`Keq`	S	Thermal conductivity (equiv)	$[\Sigma(\theta_{Pi}K_{Pi})+\Sigma(\theta_{Li}K_{Li})]/$ $[\Sigma\theta_{Pi}+\Sigma\theta_{Li}]$
S, PM	`Keq`*xixj*	S	Thermal conductivity, x_ix_j component	$K_{\mathrm{eq}ij}$
S, PM	`QH`	S	Heat source (general)	Q_H
S, PM	`QG`	S	Heat source (geothermal)	$\rho_\mathrm{geo}q_\mathrm{geo}$ (uniform) $\rho_\mathrm{geo}q_\mathrm{geo}\exp(z_\mathrm{geo}/h_\mathrm{geo})$ (exponential)

TABLE 7-4: VARIABLES IN THE CONDUCTION APPLICATION MODE

ANALYSIS	NAME	TYPE	DESCRIPTION	EXPRESSION
S, PM	`QC`	S	Convective heat source	$h_{\mathrm{trans}}(T_{\mathrm{ext}} - T)$
S, PM	`QR`	S	Radiative heat source	$C_{\mathrm{trans}}(T^4{}_{\mathrm{ambtrans}} - T^4)$
S, PM	`T`	S/B/E/P	Temperature	T
S, PM	`gradT`	S/B/E/P	Temperature gradient, norm	$\lvert\nabla T\rvert$
S, PM	`T`*xi*	V	Temperature gradient, x_i component	$\frac{\partial T}{\partial x_i}$
S, PM	`flux`	S/B/E/P	Total heat flux	$\lvert -K_{\mathrm{eq}}\nabla T\rvert$
S, PM	`flux`*xi*	V	Heat flux, x_i component	$\sum_j -K_{\mathrm{eq}ij}\frac{\partial T}{\partial x_j}$
S, PM	`nflux`	B	Normal heat flux	$\mathbf{n} \cdot (-K_{\mathrm{eq}}\nabla T)$
PM	`thetaL`	S/B/E/P	Total volume fraction (fluids)	$\Sigma\theta_{Li}$
PM	`CL`	S/B/E/P	Volume heat capacity (fluids)	$\Sigma(\theta_{Li}\,\rho_{Li}\,C_{PLi})/\Sigma\theta_{Li}$
PM	`KL`	S/B/E/P	Thermal conductivity (fluids)	$\Sigma(\theta_{Li}K_{Li})/\Sigma\theta_{Li}$
S, PM	`thetaP`	S/B/E/P	Total volume fraction (solids)	$\Sigma\theta_{Pi}$
S, PM	`CP`	S/B/E/P	Volume heat capacity (solids)	$\Sigma(\theta_{Pi}\rho_{Pi}C_{pPi})/\Sigma\theta_{Pi}$
S, PM	`KP`	S/B/E/P	Thermal conductivity (solids)	$\Sigma(\theta_{Pi}K_{Pi})/\Sigma\theta_{Pi}$
S, PM	`rhogeo`	S/B/E/P	Geothermal density	$\Sigma(\theta_{Pi}\rho_{Pi})/\Sigma\theta_{Pi}$ (solid) $[\Sigma(\theta_{Pi}\rho_{Pi})+\theta_L\rho]/(\theta_P+\theta_L)$ (porous media) (or user entry)

Note: Append an underscore plus the application mode name (default: eshc) to the application mode names in the list above, except for the dependent variable (temperature). For example, `flux_eshc` is the variable for the total heat flux.

Convection and Conduction

This application mode is for analyses involving heat transport by convection and conduction in porous media as well as free fluids. If your model contains zones with zero velocity, you still can use this application mode by setting the velocity to zero. For each instance of the application mode in your model, there is assumed to be one mobile fluid and possibly multiple other constituents whose motion is not described explicitly (for example, immobile fluids and solids). In this way, the application mode covers heat transfer in saturated and variably saturated porous media as well as convection and conduction for a single fluid. The dependent variable is temperature T. As such, enter `T` in an edit field to reference the temperature, `Tx` to state temperature gradient in the x direction, and `Tt` to see the temperature change in time. A suffix is used to designate the coefficients and other application mode variables associated with the equation. By default the suffix relates to the application mode name. For the Convection and Conduction application mode the suffix is `_eshcc`. To access the equivalent heat capacity in an equation or for postprocessing, for example, enter `Keq_eshcc` in an edit field or in your code.

PDE Formulation

The equation governing heat transfer by convection and conduction reads:

$$\delta_{\mathrm{ts}} C_{\mathrm{eq}} \frac{\partial T}{\partial t} + \nabla \cdot (-K_{\mathrm{eq}} \nabla T) = -C_L \mathbf{u} \cdot \nabla T + Q_H + Q_G$$

Application Mode Properties

The **Application Mode Properties** dialog box available in the **Physics** menu or from the **Model Navigator** provides options for the materials in the model: (1) **Mobile fluid, solid**, (2) **Immobile/mobile fluid, solid**, (3) **Mobile fluid**. The **Mobile fluid, solid** option triggers a table in the **Subdomain Settings** dialog box that allows inputs for one moving fluid and up to five solids. The **Immobile/mobile fluid, solid** option adds five more immobile components (presumably fluids) to the model. With the **Mobile fluid** option, the table provides inputs for one moving fluid.

Subdomain Settings

The **Subdomain Settings** dialog box contains the following pages:

- **Materials**
- **Time/Convection**
- **Spreading**
- **Sources/Sinks**
- **Init**
- **Element**

MATERIALS

The **Materials** page contains edit fields to input thermal properties for the different fluids and solids in your model. The table is optional except for fluids-only models. Here, you enter all thermal properties on the **Materials** page.

For models with solid constituents, the software reads the information in the table and calculates any or all of the following C_{eq}, K_{eq}, and ρ_{geo}. Depending on the application properties you select, the table may include the following:

SYMBOL	VARIABLE	DESCRIPTION
θ_L	`thetaL`	Volume fraction, mobile fluid
ρ_L	`rhoL`	Density, mobile fluid
C_{pL}	`CpL`	Specific heat capacity, mobile fluid
K_L	`KL`	Thermal conductivity, mobile fluid
θ_G	`thetaG`	Volume fraction, immobile fluid
ρ_G	`rhoG`	Density, immobile fluid
C_{pG}	`CpG`	Specific heat capacity, immobile fluid
K_G	`KG`	Thermal conductivity, immobile fluid
θ_P	`thetaP`	Volume fraction, solid
ρ_P	`rhoP`	Density, solid
C_p	`CpP`	Specific heat capacity, solid
K_P	`KP`	Thermal conductivity, solid

TIME/CONVECTION

The **Time/Convection** page is where you set up how to calculate equivalent heat capacity, the heat capacity of the mobile fluid, and the fluid velocity. The fluid velocity can be the dependent variable from another COMSOL application mode, an expression, or set to zero.

SYMBOL	VARIABLE	DESCRIPTION	OPTIONS
δ_{ts}	`Dts`	Scaling coefficient, time	
C_{eq}	`Ceq`	Volume heat capacity, Porous medium	(1) calculated, volume average (2) user defined
C_L	`CL`	Volume heat capacity, Mobile fluid	(1) calculated, volume average (2) user defined
u, v, w	`u`, `v`, `w`	Velocity components	

SPREADING

The **Spreading** page sets up equivalent thermal conductivity for the fluid-solid systems but does not appear for fluids-only models. Equivalent thermal conductivity can be defined with the following laws: (1) **Power law**, (2) **Dispersion and conduction**, (3) **Volume average**, and (4) **User defined**. The available terms in all methods are given in the table below. Details for the different options are described subsequently.

TERM	VARIABLE	DESCRIPTION
K_{eq}	`Keq`	Equivalent thermal conductivity
A_r	`Ar`	Anisotropy ratios
K_{Disp}	`KDisp`	Thermal dispersion
$\lambda_1, \lambda_2, \lambda_3$	`lambda1`, `lambda2`, `lambda3`	Thermal dispersivity, x_i direction
K_{PM}	`KPM`	Thermal conductivity, Porous Medium
A_{rPM}	`ArPM`	Anisotropy ratio, Therm Cond PM Tensor

The **Power law** option is an automatic calculation based on property expressions entered in the **Materials** page multiplied by a tensor of anisotropy ratios as follows:

$$K_{eq} = K_L^{\theta_L} K_P^{(1-\theta_L)}$$

The **Dispersion and conduction** option is analogous to spreading of pollutants described by hydrodynamic dispersion in the solute transport application modes. It combines dispersion or spreading by fluid velocity with conductive heat transfer of the porous medium as follows:

$$K_{eq} = K_{Disp} + K_{PM}$$

The **Volume average** option defines the equivalent thermal conductivity as

$$K_{\mathrm{eq}} = \frac{K_L\theta_L + K_P\theta_P + K_G\theta_G}{\theta_L + \theta_P + \theta_G}$$

By selecting **User defined** you can define the dispersion tensor K_{Disp} by specifying an expression or COMSOL result to give the spatial distribution for the dispersion coefficient and choose to multiply by a tensor of anisotropy ratios A_{r} if desired. Or you can provide information about longitudinal λ_1 and transverse λ_2 and λ_3 dispersivities that will be used to calculate the tensor using the fluid velocities as follows.

The **User defined** option also consists of the expression you enter multiplied by a tensor of anisotropy ratios.

For 3D models with u, v, and w as directional velocities, the K_{Disp} tensor entries are:

SYMBOL	VARIABLE	EXPRESSION
K_{Disp11}	`KDisp11`	$C_L(\lambda_1 u^2 + \lambda_2 v^2 + \lambda_3 w^2)/U^2$
K_{Disp12}	`KDisp12`	$(\lambda_1 - \lambda_2)C_L uv/U$
K_{Disp13}	`KDisp13`	$(\lambda_1 - \lambda_3)C_L uw/U$
K_{Disp21}	`KDisp21`	K_{Disp12}
K_{Disp22}	`KDisp22`	$C_L(\lambda_1 v^2 + \lambda_2 u^2 + \lambda_3 w^2)/U^2$
K_{Disp23}	`KDisp23`	$(\lambda_2 - \lambda_3)C_L vw/U$
K_{Disp31}	`KDisp31`	K_{Disp13}
K_{Disp32}	`KDisp32`	K_{Disp23}
K_{Disp33}	`KDisp33`	$C_L(\lambda_1 w^2 + \lambda_2 u^2 + \lambda_3 v^2)/U^2$

For 2D models with u and v as directional velocities, the K_{Disp} tensor entries are:

SYMBOL	VARIABLE	DEFINITION
K_{Disp11}	`KDisp11`	$C_L(\lambda_1 u^2 + \lambda_2 v^2)/U^2$
K_{Disp12}	`KDisp12`	$(\lambda_1 - \lambda_2)C_L uv/U$
K_{Disp21}	`KDisp21`	K_{Disp12}
K_{Disp22}	`KDisp22`	$C_L(\lambda_1 v^2 + \lambda_2 u^2)/U^2$

In 1D K_{Disp} is:

SYMBOL	VARIABLE	DEFINITION
K_{Disp11}	`KDisp11`	$C_L\lambda_1 u^2/U^2$

SOURCES/SINKS

The **Sources/Sinks** page is identical to the one shown in the Conduction application mode except for the following points: (1) the list box for **Geothermal density** does not appear for systems involving fluids only, and (2) the convective and radiative source terms Q_C and Q_R, respectively, do not appear in the Convection and Conduction application mode. For details, see the description of the Conduction application mode.

Boundary Settings

The boundary conditions set out in the following table are available.

TYPE	BOUNDARY CONDITION	DESCRIPTION
T	$T = T_0$	Temperature
N0	$-\mathbf{n}\cdot\mathbf{N} = N_0$ $\mathbf{N} = -K_{\mathrm{eq}}\nabla T + C_L\mathbf{u}T$	Heat Flux
Nz	$-\mathbf{n}\cdot\mathbf{N} = 0$ $\mathbf{N} = -K_{\mathrm{eq}}\nabla T + C_L\mathbf{u}T$	Thermal insulation
Nc	$-\mathbf{n}\cdot K_{\mathrm{eq}}\nabla T = 0$	Convective flux
ax	$-\mathbf{n}\cdot\mathbf{N} = 0$ $\mathbf{N} = -K_{\mathrm{eq}}\nabla T + C_L\mathbf{u}T$	Axial symmetry

Note that the axial symmetry condition is identical to the insulation/symmetry condition and is only available for axisymmetric models.

Point Settings, Edge Settings, and Scalar Variables

The **Point Settings**, **Edge Settings**, and **Scalar Variables** dialog boxes are described for the Conduction application mode.

Application Mode Variables

Table 7-5 lists the application mode variables for the Convection and Conduction application mode. In the Analysis column MF stands for Mobile fluid, MF/S for Mobile fluid, solid and MF/IF/S for Mobile/immobile fluid, solid.

TABLE 7-5: VARIABLES IN THE CONVECTION AND CONDUCTION APPLICATION MODE

ANALYSIS	Name	**TYPE**	**DESCRIPTION**	**EXPRESSION**
	`Dts`	S/B/E/P	Time scaling coefficient	δ_{ts}
MF/S	`Ceq`	S/B/E/P	Volume heat capacity (equivalent)	$\frac{\theta_L C_L + \theta_P C_P}{\theta_L + \theta_P}$ (or user entry)
MF/IF/S	`Ceq`	S/B/E/P	Volume heat capacity (equivalent)	$\frac{\theta_L C_L + \theta_G C_G + \theta_P C_P}{\theta_L + \theta_G + \theta_P}$ (or user entry)
MF	`Ceq`	S/B/E/P	Volume heat capacity (equivalent)	$C_{\mathrm{eq}} = C_L$
All	`CL`	S/B/E/P	Volume heat capacity (mobile fluid)	$\rho_L C_{PL}$ (or user entry)
MF/S	`Keq`	S/B/E/P	Thermal conductivity (equivalent)	$K_L \theta_L K_P^{(1-\theta_L)}$ (power law) $\frac{K_L \theta_L + K_P \theta_P}{\theta_L + \theta_P}$ (volume average) $K_{\mathrm{Disp}} + K_{PM}$ (disp. and cond.) (or user entry)
MF/IF/S	`Keq`	S/B/E/P	Thermal conductivity (equivalent)	$K_L \theta_L K_P^{(1-\theta_L)}$ (power law) $\frac{K_L \theta_L + K_P \theta_P + K_G \theta_G}{\theta_L + \theta_P + \theta_G}$ (volume average) $K_{\mathrm{Disp}} + K_{PM}$ (disp. and cond.) (or user entry)
All	`Keq`*`xixj`*	S/B/E/P	Thermal conductivity (equivalent)	$A_r K_{\mathrm{eq}}$

TABLE 7-5: VARIABLES IN THE CONVECTION AND CONDUCTION APPLICATION MODE

ANALYSIS	Name	**TYPE**	**DESCRIPTION**	**EXPRESSION**
MF	Keq	S/B/E/P	Thermal conductivity (equivalent)	K_L
MF/S	KPM	S/B/E/P	Thermal conductivity (porous media)	$\frac{(\theta_L K_L + \theta_P K_P)}{\theta_L + \theta_P}$ (or user entry)
MF/IM/S	KPM	S/B/E/P V	Thermal conductivity (porous media)	$\frac{K_L \theta_L + K_P \theta_P + K_G \theta_G}{\theta_L + \theta_P + \theta_G}$ (or user entry)
	u, v, w	S/B/E/P/V	Velocity u, v, w in x_i direction	u, v, w
	U	S/B/E/P	Velocity U	$\lvert\mathbf{u}\rvert$
	QH	S	Heat source (general)	Q_H
All	QG	S	Heat source (geothermal)	$\rho_{\mathrm{geo}} q_{\mathrm{geo}}$ (uniform heat prod.) $\rho_{\mathrm{geo}} q_{\mathrm{geo}} h_{\mathrm{geo}} \exp(z_{\mathrm{geo}}/h_{\mathrm{geo}})$ (exponential heat prod.) (or user entry)
All	T	S/B/E/P	Temperature	T
All	gradT	S/B/E/P	Temperature gradient, norm	$\lvert\nabla T\rvert$
All	T*xi*	V	Temperature gradient, x_i component	$\frac{\partial T}{\partial x_i}$
MF/S, MF/IF/S	tflux	S/B/E/P	Total heat flux, norm	$\lvert -K_{\mathrm{eq}} \nabla T + C_L \mathbf{u} T\rvert$
MF/S, MF/IF/S	tflux*xi*	V	Total heat flux, x_i component	$(-K_{\mathrm{eq}} \nabla T + C_L \mathbf{u} T)_i$
MF	tflux	S/B/E/P	Total heat flux, norm	$\lvert K_{\mathrm{eq}} \nabla T\rvert$
MF	tflux*xi*	V	Total heat flux, x_i component	$-K_{\mathrm{eq}} (\nabla T)_i$
All	dtflux	S/B/E/P	Total diffusive flux, norm	$\lvert K_{\mathrm{eq}} \nabla T\rvert$
All	dtflux*xi*	V	Total diffusive flux, x_i component	$-K_{\mathrm{eq}} (\nabla T)_i$
MF/S, MF/IF/S	diflux	S/B/E/P	Dispersive flux, norm	$\lvert K_{\mathrm{Disp}} \nabla T\rvert$

TABLE 7-5: VARIABLES IN THE CONVECTION AND CONDUCTION APPLICATION MODE

ANALYSIS	Name	TYPE	DESCRIPTION	EXPRESSION
MF/S, MF/IF/S	`difluxxi`	V	Dispersive flux, x_i component	$-K_{\mathrm{Disp}}(\nabla T)_i$
MF/S, MF/IF/S	`dflux`	S/B/E/P	Total conductive flux, norm	$\lvert K_{\mathrm{PM}}\nabla T\rvert$
MF/S, MF/IF/S	`dfluxxi`	V	Total conductive flux, x_i component	$-K_{\mathrm{PM}}(\nabla T)_i$
All	`cflux`	S/B/E/P	Convective flux, norm	$\lvert C_L\mathbf{u}T\rvert$
All	`cfluxxi`	V	Convective flux, x_i component	$C_L u_i T$
MF/S, MF/IF/S	`ntflux`	B	Normal total heat flux	$\mathbf{n}\cdot(-K_{\mathrm{eq}}\nabla T+C_L\mathbf{u}T)$
MF	`ntflux`	B	Normal total flux	$\mathbf{n}\cdot(-K_{\mathrm{eq}}\nabla T)$
MF/S, MF/IF/S	`ndtflux`	B	Normal total diffusive flux	$\mathbf{n}\cdot(-K_{\mathrm{eq}}\nabla T)$
MF/S, MF/IF/S	`ndiflux`	B	Normal dispersive flux	$\mathbf{n}\cdot(-K_{\mathrm{Disp}}\nabla T)$
MF/S, MF/IF/S	`ndflux`	B	Normal total conductive flux	$\mathbf{n}\cdot(-K_{\mathrm{PM}}\nabla T)$
All	`thetaL`	S/B/E/P	Total volume fraction (mobile fluid)	θ_L
All	`CL`	S/B/E/P	Volume heat capacity (mobile fluid)	$\theta_L\rho_L C_{PL}$
All	`KL`	S/B/E/P	Thermal conductivity (mobile fluid)	K_L
MF/IM/S	`thetaG`	S/B/E/P	Total volume fraction (immobile fluid)	$\Sigma\theta_{Gi}$
MF/IM/S	`CG`	S/B/E/P	Volume heat capacity (immobile fluid)	$\Sigma(\theta_{Gi}\rho_{Gi}C_{pGi})/\Sigma\theta_{Gi}$
MF/IM/S	`KG`	S/B/E/P	Thermal conductivity (immobile fluid)	$\Sigma(\theta_{Gi}K_{Gi})/\Sigma\theta_{Gi}$
MF/S, MF/IF/S	`thetaP`	S/B/E/P	Total volume fraction (solids)	$\Sigma\theta_{Pi}$
MF/S, MF/IF/S	`CP`	S/B/E/P	Volume heat capacity (solids)	$\Sigma(\theta_{Pi}\rho_{Pi}C_{pPi})/\Sigma\theta_{Pi}$

TABLE 7-5: VARIABLES IN THE CONVECTION AND CONDUCTION APPLICATION MODE

ANALYSIS	Name	**TYPE**	**DESCRIPTION**	**EXPRESSION**
MF/S, MF/IF/S	`KP`	S/B/E/P	Thermal conductivity (solids)	$\Sigma(\theta_{Pi}K_{Pi})/\Sigma\theta_{Pi}$
MF/S, MF/IF/S	`lambda1`, `lambda2`, `lambda3`	S/B/E/P/V	Thermal dispersivity in x_1, x_2, x_3 direction	λ_1, λ_2, λ_3
MF/S	`rhogeo`	S/B/E/P	Geothermal density	$\Sigma(\theta_{Pi}\rho_{Pi})/\Sigma\theta_{Pi}$ (solid) $(\Sigma(\theta_{Pi}\rho_{Pi})+\theta_L\rho)/(\theta_P+\theta_L)$ (porous media) (or user entry)
MF/IF/S	`rhogeo`	S/B/E/P	Geothermal density	$\Sigma(\theta_{Pi}\rho_{Pi})/\Sigma\theta_{Pi}$ (solid) $(\Sigma(\theta_{Pi}\rho_{Pi})+\theta_L\rho+\Sigma(\theta_{Gi}\rho_{Gi}))/$ $(\theta_P+\theta_G+\theta_L)$ (porous media) (or user entry)
MF	`rhogeo`	S/B/E/P	Geothermal density	ρ_{geo}
All	`cellPe`	S	Cell Peclet number	$\left\lvert\frac{\mathbf{u}h}{K_{\text{eq}}}\right\rvert$
All	`qgeo`	S/B/E/P	Radiogenic heating per mass	q_{geo}
All	`zgeo`	S/B/E/P	Depth	z_{geo}
All	`hgeo`	S/B/E/P	Length scale	h_{geo}

Note: Append an underscore plus the application mode name (default: eshcc) to the application mode names in the list above, except for the dependent variable (temperature). For example, `tflux_eshcc` is the variable for the norm of the total heat flux.

Solute Transport

This application mode can be used for isothermal solute transport by advection, dispersion, sorption, and volatilization in saturated porous media. Frequently used reaction terms are included. The application mode is available for 1D, 2D, 3D, and axisymmetric systems in 1D, and 2D. Dependent variables are dissolved concentrations: $c_1, c_2, \ldots, c_n$.

PDE Formulation

The governing equation for saturated media is as follows:

$$\delta_{\mathrm{ts1}}\left(\theta + \rho_{\mathrm{b}}\frac{\partial c_{Pi}}{\partial c} + a_v\frac{\partial c_{Gi}}{\partial c}\right)\frac{\partial c}{\partial t} + \delta_{\mathrm{ts2}}(1 - k_G)c\frac{\partial \theta}{\partial t} + \nabla \cdot [-\theta D_{LGi}\nabla c_i + \mathbf{u}c_i] = R_{Li} + R_{Pi} + R_{Gi} + S_{ci}$$

Here, c_i, $c_{Pi,}$ and c_{Gi} denote the solute concentration in the liquid (mass per liquid volume), that sorbed to solid particles (mass per dry unit weight of the solid), and the solute concentration in the gas for species i, respectively. Furthermore, θ, termed the *porosity*, is the volume of fluids divided by the total fluid-solid volume; $\rho_{\mathrm{b}} = (1 - \theta)\rho_p$ is the bulk density of the porous medium when ρ_p is the particle density; D_{LGi} represents the hydrodynamic and gas dispersion tensor; $\mathbf{u}$ is the vector of directional velocities; R_{Li}, R_{Pi}, and R_{Gi} describe reactions in the liquid, solid and gas phases, respectively, and S_{ci} denotes a solute source.

The above equation is the conservative form of the equation. Assuming that the velocity is divergence free, the nonconservative form can be derived.

$$\delta_{\mathrm{ts1}}\left(\theta + \rho_{\mathrm{b}}\frac{\partial c_{Pi}}{\partial c} + a_v\frac{\partial c_{Gi}}{\partial c}\right)\frac{\partial c}{\partial t} + \delta_{\mathrm{ts2}}(1 - k_G)c\frac{\partial \theta}{\partial t} + \nabla \cdot [-\theta D_{LGi}\nabla c_i] = -\mathbf{u}\nabla c_i + R_{Li} + R_{Pi} + R_{Gi} + S_{ci}$$

Subdomain Settings

The **Subdomain Settings** dialog box contains the following pages:

- **Flow and Media**
- **Liquid**

- **Solid**
- **Gas**
- **Init**
- **Element**

In the **Application Mode Properties** dialog box you can choose between liquid transport only; liquid and solid; liquid, solid, and gas; or liquid and gas. Only the tabs needed for the chosen material property will be available and when only liquid is chosen the **Liquid** tab is instead called **Solute**.

FLOW AND MEDIA

The **Flow and Media** page includes the following coefficients.

SYMBOL	VARIABLE	DESCRIPTION	OPTION
δ_{ts1}	`Cts1`	Time scaling coefficient 1	
θ	`theta`	Liquid volume fraction	
θ_s	`theta_s`	Pure volume fraction	
u, v, w	`u`, `v`, `w`	Darcy velocity in the x_1, x_2, and x_3 directions	
Q_s	`Qs`	Fluid source	
δ_{ts2}	`Cts2`	Time-scaling coefficient 2	
	`fractiontype`	Time change in liquid volume fraction	(1) Coupled pressure head (2) Time change in pressure head (3) Time change in fluid fraction (4) Fluid fraction constant with time
C	`C`	Specific moisture capacity	
dH_p/dt	`dHpdt`	Time change in pressure head	
$d\theta/dt$	`dthdt`	Time change in fluid fraction	

$\theta = \theta_s$ if the material property does not contain gas.

LIQUID/SOLUTE

The **Liquid/Solute** page includes the following coefficients.

SYMBOL	VARIABLE	DESCRIPTION
α_1	`alpha1`	Dispersivity, x_1 direction
α_2	`alpha2`	Dispersivity, x_2 direction
α_3	`alpha3`	Dispersivity, x_3 direction

SYMBOL	VARIABLE	DESCRIPTION
	`tauLtype`	(1) Computed (2) User defined
τ_L	`tauL`	Tortuosity factor
D_{mL}	`DmL`	Coefficient of molecular diffusion
R_L	`RL`	Reaction rate, liquid
c_Q	`cQ`	Fluid source concentration
S_o	`So`	Other solute source

SOLID

On the **Solid** page, the following coefficients are available:

SYMBOL	VARIABLE	DESCRIPTION	OPTIONS
	`sorptiontype`	Sorption isotherms	(1) Freundlich (2) Langmuir (3) User defined
ρ_b	`rhob`	Bulk density	
N	`NF`	Freundlich exponent	
K_F	`KF`	Freundlich constant	
K_L	`KL`	Langmuir constant	
$\bar{s}$	`sbarL`	Langmuir sorption maximum	
K_P	`KP`	User defined isotherm	
R_P	`RP`	Reaction rate, solid	

GAS

On the **Gas** page, the following coefficients are available:

SYMBOL	VARIABLE	DESCRIPTION	OPTION
K_G	`KG`	Isotherm volatilization	
	`tauGtype`	Gas phase tortuosity type	Calculated User defined
τ_G	`tauG`	Gas phase tortuosity	
D_{mG}	`DmG`	Molecular diffusion coefficient, gas	
	`Artype`	Anisotropy	On Off

SYMBOL	VARIABLE	DESCRIPTION	OPTION
A_{r}	`Ar`	Diffusion anisotropy tensor	
R_G	`RG`	Reaction rate, gas	

Boundary Settings

The available boundary conditions are as follows:

TYPE	BOUNDARY CONDITION	DESCRIPTION
C	$c = c_0$	Concentration
N0	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c + \mathbf{u}c) = N_0$	Flux
Nn	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c + \mathbf{u}c) = 0$	No flux/Symmetry
Na	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c) = 0$	Advective flux
Nd	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c) = N_0$	Dispersive flux
Ngen	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c + \mathbf{u}c) = \mathbf{n}\cdot\mathbf{u}c_0 + N_0$	General Neumann expression
NGatmf	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c + \mathbf{u}c) = N$ $N = \mathbf{n}\cdot\mathbf{u}c_0 - \frac{D_{mG}}{d}(k_G c - c_{G\mathrm{atm}})$	Flow boundary volatilization
NnGatmz	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c + \mathbf{u}c) = N$ $N = -\frac{D_{mG}}{d}(k_G c - c_{G\mathrm{atm}})$	No flow boundary volatilization
ax	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c + \mathbf{u}c) = 0$	Axial symmetry (axisymmetric models only)

Point Settings and Edge Settings

Point Settings (2D and 3D) and Edge Settings (3D) are given in the following table. Options for both stationary and time-dependent inputs are available. In time-dependent simulations, the point may switch from a specified *c* to a specified flux.

If both c and a flux are specified on the same point or edge for the same time, the specified concentration will be simulated, and the specified flux will be neglected.

SYMBOL	**VARIABLE**	**ANALYSIS**	**DESCRIPTION**
c_0	`c0`	stationary	Concentration
c_0	`c0`	transient	Concentration
t_{c0}	`tc0`	transient	Starting time, Concentration
t_{cf}	`tcf`	transient	Ending time, Concentration
N_0	`N0`	stationary	Flux
N_0	`N0`	transient	Flux
t_{N0}	`tN0`	transient	Starting time, flux
t_{Nf}	`tNf`	transient	Ending time, flux

Application Mode Variables

The following variables are available to use in the equation or in postprocessing.

TABLE 7-6: VARIABLES IN THE SOLUTE TRANSPORT APPLICATION MODE

NAME	**MAT TYPE**	**TYPE**	**DESCRIPTION**	**EXPRESSION**
`thDLxx_c`	All	S/B/E/P	Dispersive tensor, xx component	$\alpha_1\frac{u^2}{\lvert\mathbf{u}\rvert}+\alpha_2\frac{v^2}{\lvert\mathbf{u}\rvert}+\alpha_3\frac{w^2}{\lvert\mathbf{u}\rvert}+\theta\tau_L D_m$
`thDLxy_c`	All	S/B/E/P	Dispersive tensor, xy component	$(\alpha_1-\alpha_2)\frac{uv}{\lvert\mathbf{u}\rvert}$
`thDLxz_c`	All	S/B/E/P	Dispersive tensor, xz component	$(\alpha_1-\alpha_3)\frac{uw}{\lvert\mathbf{u}\rvert}$
`thDLyx_c`	All	S/B/E/P	Dispersive tensor, yx component	$(\alpha_1-\alpha_2)\frac{uv}{\lvert\mathbf{u}\rvert}$
`thDLyy_c`	All	S/B/E/P	Dispersive tensor, yy component	$\alpha_1\frac{v^2}{\lvert\mathbf{u}\rvert}+\alpha_2\frac{u^2}{\lvert\mathbf{u}\rvert}+\alpha_3\frac{w^2}{\lvert\mathbf{u}\rvert}+\theta\tau_L D_m$
`thDLyz_c`	All	S/B/E/P	Dispersive tensor, yz component	$(\alpha_1-\alpha_3)\frac{vw}{\lvert\mathbf{u}\rvert}$
`thDLzx_c`	All	S/B/E/P	Dispersive tensor, zx component	$(\alpha_1-\alpha_3)\frac{uw}{\lvert\mathbf{u}\rvert}$
`thDLzy_c`	All	S/B/E/P	Dispersive tensor, zy component	$(\alpha_1-\alpha_3)\frac{vw}{\lvert\mathbf{u}\rvert}$

TABLE 7-6: VARIABLES IN THE SOLUTE TRANSPORT APPLICATION MODE

NAME	MAT TYPE	TYPE	DESCRIPTION	EXPRESSION
thDLzz_c	All	S/B/E/P	Dispersive tensor, *zz* component	$\alpha_1\frac{w^2}{\lvert\mathbf{u}\rvert}+\alpha_3\frac{u^2}{\lvert\mathbf{u}\rvert}+\alpha_3\frac{v^2}{\lvert\mathbf{u}\rvert}+\theta\tau_L D_m$
thDLG*ij*_c	G	S/B/E/P	Liquid Gas Dispersive tensor	$\theta D_{Lij}+a_v D_{Gij}$
avDG*ij*_c	G	S/B/E/P	Gas Diffusion tensor	$a_v\tau_G D_{mG} A_{rij} k_G$
kP_c	S	S/B/E/P	Isotherm sorption	$K_F c^{(N_F-1)}$ (Freundlich) $\frac{K_L\bar{s}}{1+K_L}$ (Langmuir) K_P (User defined)
dcP_c	S	S/B/E/P	Sorption derivative	$N_F K_F c^{(N_F-1)}$ (Freundlich) $\frac{K_L\bar{s}}{(1+K_L)^2}$ (Langmuir) $\frac{\partial}{\partial c}Kc$ (User defined)
cP_c	S	S/B/E/P	Concentration solid	ck_P
kG_c	G	S/B/E/P	Isotherm volatilization	K_G
cG_c	G	S/B/E/P	Concentration gas	
c	All	S/B/E/P	Concentration	c
grad_c_*xi*	All	V	Concentration gradient, x_i component	$\frac{\partial c}{\partial x_i}$
grad_c	All	S/B/E/P	Concentration gradient, norm	$\lvert\nabla c\rvert$
u, v, w	All	V	Darcy velocity, x_i component	u, v, w
U	All	S/B/E/P	Darcy velocity, norm	$\sqrt{u^2+v^2+w^2}$
av	G	S/B/E/P	Gas volume fraction	$a_v=\theta_s-\theta$
ua, va, wa	All	V	Average linear velocity, x_i component	$\frac{u}{\theta}$, $\frac{v}{\theta}$, $\frac{w}{\theta}$
Ua	All	S/B/E/P	Average linear velocity, norm	$\sqrt{u_a^2+v_a^2+w_a^2}$

TABLE 7-6: VARIABLES IN THE SOLUTE TRANSPORT APPLICATION MODE

NAME	MAT TYPE	TYPE	DESCRIPTION	EXPRESSION
`RF_c`	S, G	S/B/E/P	Retardation factor	$1+\frac{\rho_b}{\theta}k_P$ (no gas) $1+\frac{a_v}{\theta}k_G$ (no solid) $1+\frac{\rho_b}{\theta}k_P+\frac{a_v}{\theta}k_G$
`uR_c`, `vR_c`, `wR_c`	S, G	V	Retarded velocity, x_i component	$\frac{u_a}{R_F}, \frac{v_a}{R_F}, \frac{w_a}{R_F}$
`cellPe_c`	All	S/B/E/P	Cell Peclet number	$\left\lvert\frac{\mathbf{u}h}{\theta D_L}\right\rvert$ (no gas) $\left\lvert\frac{\mathbf{u}h}{\theta D_{LG}}\right\rvert$ (gas)
`dflux_c_xi`	All	V	Dispersive flux, x_i component	$-\theta D_{LG}\frac{\partial c}{\partial x_i}$ (gas) $-\theta D_L\frac{\partial c}{\partial x_i}$ (no gas)
`dflux_c`	All	S/B/E/P	Dispersive flux, norm	$\lvert\theta D_L\nabla c\rvert$ (no gas) $\lvert\theta D_{LG}\nabla c\rvert$ (gas)
`dLflux_c_xi`	G	V	Dispersive flux, liquid, x_i component	$-\theta D_L\frac{\partial c}{\partial x_i}$
`dLflux_c`	G	S/B/E/P	Dispersive flux, liquid, norm	$\lvert\theta D_L\nabla c\rvert$
`dGflux_c_xi`	G	V	Dispersive flux, gas, x_i component	$-a_v D_G\frac{\partial c}{\partial x_i}$
`dGflux_c`	G	S/B/E/P	Dispersive flux, gas, norm	$\lvert a_v D_G\nabla c\rvert$
`adflux_c_xi`	All	V	Advective flux, x_i component	cu, cv, cw
`adflux_c`	All	S/B/E/P	Advective flux, norm	$\lvert c\mathbf{u}\rvert$

TABLE 7-6: VARIABLES IN THE SOLUTE TRANSPORT APPLICATION MODE

NAME	**MAT TYPE**	**TYPE**	**DESCRIPTION**	**EXPRESSION**
`tflux_c_xi`	All	V	Total flux, x_i component	$-\theta D_L \frac{\partial c}{\partial x_i} + c u_i$
`tflux_c`	All	S/B/E/P	Total flux, norm	$\lvert -\theta D_L \nabla c + c\mathbf{u} \rvert$
`ndflux_c`	All	B	Normal dispersive flux	$-\mathbf{n} \cdot \theta D_L \nabla c$ (no gas) $-\mathbf{n} \cdot \theta D_{LG} \nabla c$ (gas)
`nadflux_c`	All	B	Normal advective flux	$\mathbf{n} \cdot c\mathbf{u}$
`ntflux_c`	All	B	Normal total flux	$\mathbf{n} \cdot (-\theta D_L \nabla c + c\mathbf{u})$ (no gas) $\mathbf{n} \cdot (-\theta D_{LG} \nabla c + c\mathbf{u})$ (gas)

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