COMSOL
MULTIPHYSICS

EARTH SCIENCE MODULE

USER'S GUIDE

VERSION 3.4

COMSOL

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Earth Science Module User's Guide

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1

Introduction

The Earth Science Module is an extension of COMSOL Multiphysics for simulation of subsurface flow and other applications in earth science. This chapter provides an introduction to the module and an overview of its capabilities.

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 a section that presents the different application modes available in the module and discusses the modeling strategy for various test cases. The final section 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 support@comsol.com.

New Features in the Earth Science Module 3.4

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

- Interface to the COMSOL Reaction Engineering Lab, which can now export models for reaction engineering to the Solute Transport application mode for modeling of, for example, contamination of rock and soil. For an example, see the model "Pesticide Transport and Reaction in Soil" on page 265 in the *Earth Science Module Model Library.*
- Improved performance and easier-to-use boundary conditions for fluid-flow modeling using the Navier-Stokes and Brinkman equations.
- Interface to material libraries for a number of material properties in the Richards' Equation, Darcy's Law, and Convection and Conduction application modes. Click the **Load** button in the **Subdomain Settings** dialog boxes in these application modes to get access the material libraries. For more information about the use of the material libraries, see "Using the Materials/Coefficients Library" on page 223 in the *COMSOL Multiphysics User's Guide*.
- Improved Model Library with many updated models and a new model of pesticide decay and contamination.

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).

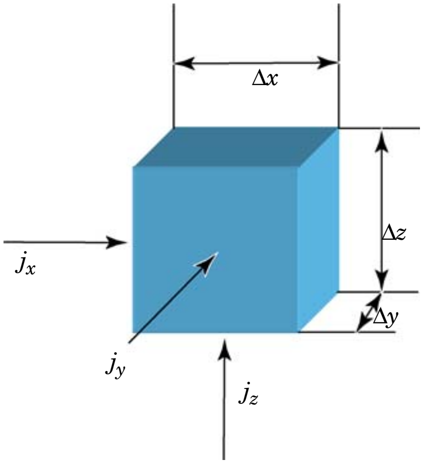
- The symbol **>** indicates a menu item or an item in a folder in the **Model Navigator**. For example, **Physics>Equation System>Subdomain Settings** is equivalent to: On the **Physics** menu, point to **Equation System** and then click **Subdomain Settings**. **COMSOL Multiphysics>Heat Transfer>Conduction** 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 COMSOL Script codes.
- 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.

Overview

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



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

In this equations the term on the left-hand side represents accumulation or the change in the amount of u stored in some time period 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.

2

The Modeling Environment

This chapter provides information about 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.

The Application Modes

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 also can them to other physics to describe poroelasticity, convection of heat and density driven flows, solute transfer, and electromagnetic forces, to name a few.
- 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 chapter that follows describes the equations and boundary conditions predefined for 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 MODE **APPLICATION MODE PROPERTY OPTIONS**	**MODE NAME**	**DEPENDENT VARIABLE**	**1D**	**2D**	**3D**	**STATIONARY**	**TRANSIENT**
FLUID FLOW							
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							
Conduction, Cartesian coordinates	eshc	T	√	√	√	√	√
Conduction, axisymmetry	eshc	T	√	√	√	√	√
Solids			√	√	√	√	√
Porous media			√	√	√	√	√
Convection and conduction, Cartesian coordinates	eshcc	T	√	√	√	√	√
Convection and conduction, axisymmetry	eshcc	T	√	√		√	√

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

APPLICATION MODE APPLICATION MODE PROPERTY OPTIONS	MODE NAME	DEPENDENT VARIABLE	1D	2D	3D	STATIONARY	TRANSIENT
Mobile fluid			√	√	√	√	√
Mobile fluid/solids			√	√	√	√	√
Mobile fluid/immobile fluid/solids			√	√	√	√	√
SOLUTE TRANSPORT							
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			√	√	√	√	√

Fluid Flow Application Modes

The catalog of fluid flow application modes in the Earth Science Module provide tools to characterize movements of liquids, gases, and other flowing media, such as molten rock. The Navier-Stokes equations describe free flows within a river or well, for example. For porous media, the Brinkman equations cover high-velocity flows; Darcy's law describes low-velocity flows of one or more fluids; and Richards' equation explains how the wetting and drying of rocks or soils. The different equations in the module 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.

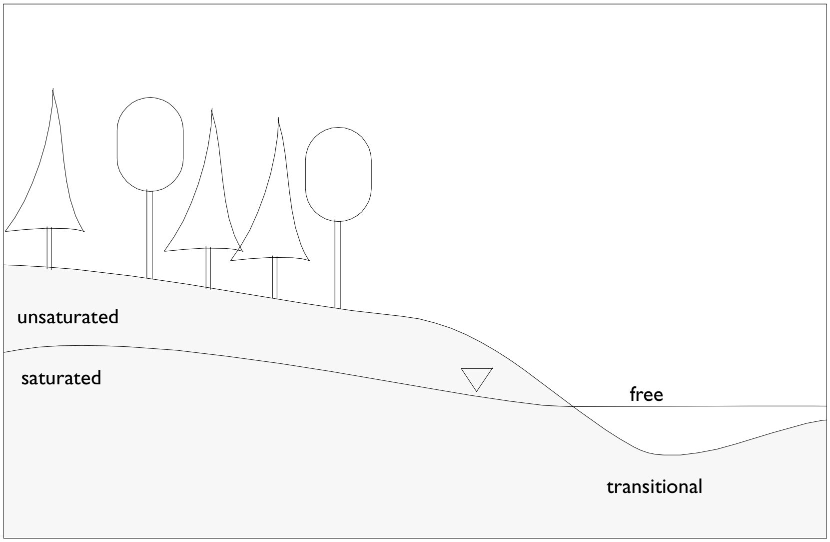


Figure 2-1: Vertical cross section through ground near a river. Labels indicate flow regimes. The triangle denotes the water table.

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 within pore velocity profiles infeasible 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 fluid velocity, ρ_f is fluid density, p is 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

The Darcy's law application mode of the Earth Science Module describes fluid movement through interstices in a porous medium. Because the fluid loses considerable energy to frictional resistance within pores, the 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 also can set up multiple Darcy's Law applications to model multiphase flows, involving more than one mobile phase.

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

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

In the equation, $\mathbf{u}$ is the Darcy velocity or specific discharge vector; κ is the permeability of the porous media; η is the fluid's dynamic viscosity; p is the fluid's pressure and ρ_f is its density; g is the magnitude of gravitational acceleration; and D is 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, $\rho_f gD$. COMSOL Multiphysics solves for the pressure, p. You set both the gravitational vector's direction, D, and magnitude, g. The choices related to gravity simplify modeling certain geometries, facilitate investigations of fluid movements on planets other than earth. By default, g equals 9.82 $\mathrm{m/s^2}$, and D is the vertical axis in the model. 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

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

$$\frac{\partial}{\partial t}(\rho_f\theta_s) + \nabla \cdot \rho_f\left[-\frac{\kappa}{\eta}(\nabla p + \rho_f g \nabla D)\right] = \rho_f \boldsymbol{Q}_s \tag{2-1}$$

where $\boldsymbol{Q}_s$ is the strength of a fluid source. 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 2-1) takes the common form shown by default in the user interface:

$$S\frac{\partial p}{\partial t} + \nabla \cdot \left[-\frac{\kappa}{\eta}(\nabla p + \rho_f g \nabla D)\right] = \boldsymbol{Q}_s \cdot$$

In the equation, S is a storage coefficient, 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.

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) where $\mathbf{u}_\alpha = \mathbf{u}/\theta_\mathrm{s}$. Here θ_s is the fluid volume fraction. For saturated systems, θ_s gives 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

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

In the equation, δ represent 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). The user 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 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

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

where N_0 is a value or expression for the flux you specify.

Occasionally you need to specify the flux into the flow domain 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

$$\mathbf{n} \cdot \frac{\kappa}{\eta}(\nabla p + \rho_f g \nabla D) = N_0 + R_b[(p_b - p) + \rho_f g(D_b - D)] \qquad \text{(2-2)}$$

where p_b and D_b are the pressure and elevation of the distant fluid source; and R_b is the "conductance" of materials between the source and the model domain. Typically $R_b = K'/B'$ where K' is the permeability of the thin layer and B' is its thickness. The stated flux N_0 can assume a value or you can set it to zero. Using logical relationships, it is possible to activate these expressions at different times or under various flow conditions.

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Darcy's Law—Head

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; and g the magnitude of gravitational acceleration. 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 media, and η is the fluid viscosity of the fluid or hydraulic conductivity, K. The hydraulic conductivity represents both fluid and solid properties.

Hydraulic Head Analysis

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

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

The governing equation becomes

$$S\frac{\partial H}{\partial t} + \nabla \cdot [-K\nabla H] = Q_s \tag{2-3}$$

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
$\mathbf{n} \cdot K\nabla H = N_0 + R_b[H_b - H]$	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.

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:

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

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
$\mathbf{n} \cdot K\nabla(H_p + D) = N_0 + R_b[(H_{pb} + D_b) - (H_p + D)]$	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 **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 systems** 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

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 that not taken up with the liquid contains an immobile fluid (air) at atmospheric pressure.

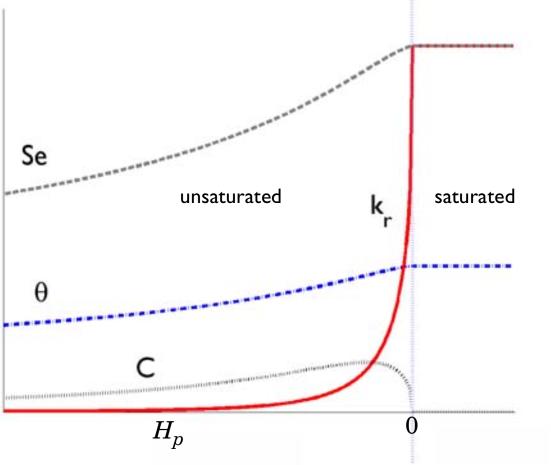

Figure 2-2: Fluid retention and permeability functions that vary with pressure head, as given by Van Genuchten formulas available in the Richards' Equation application mode.

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):

$$\delta_{ts}\left[\frac{C}{\rho_f g}+\mathrm{Se}S\right]\frac{\partial p}{\partial t}+\nabla\cdot\left[-\frac{\kappa_s}{\eta}k_r\nabla(p+\rho_f gD)\right] = Q_s$$

where pressure, p, is the dependent variable. In the equation, δ_{ts} is an optional coefficient, 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

$$\mathbf{u} = -\frac{\kappa_s}{\eta}k_r\nabla(p + \rho_f gD)$$

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 $\mathbf{u}_a = \mathbf{u}/\theta$.

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 $H_p = p/(\rho_f g)$, 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

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

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

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

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

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

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

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

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

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

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 very 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
$p = 0$	Free surface
$\mathbf{n} \cdot \frac{\kappa}{\eta} k_r (\nabla p + \rho_f g \nabla D) = 0$	Zero flux
$\mathbf{n} \cdot \frac{\kappa}{\eta} k_r (\nabla p + \rho_f g \nabla D) = 0$	Symmetry
$\mathbf{n} \cdot \frac{\kappa}{\eta} k_r (\nabla p + \rho_f g \nabla D) = N_0$	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.

References

1. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier Scientific Publishing Co, 1972.

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3. R.A. Freeze, “Three-dimensional, transient, saturated-unsaturated flow in a groundwater basin,” *Water Resour. Res.*, vol. 7, no. 2, 1971.

4. M.Th. van Genuchten, “A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils,” *Soil Sci. Soc. Am. J.*, vol. 44, 1980.

5. R.H. Brooks and A.T. Corey, “Properties of porous media affecting fluid flow,” *J. Irrig. Drainage Div., ASCE Proc.*, vol 72 (IR2), 1966.

The Brinkman Equations

The Brinkman equations describe fast moving fluids in porous media with the kinetic potential from fluid velocity, pressure, and gravity to drive the flow. These equations extend Darcy's law to describe the dissipation of the kinetic energy by viscous shear as with the Navier-Stokes 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

$$\rho\frac{\partial\mathbf{u}}{\partial t}-\nabla\cdot\frac{\eta}{\varepsilon}(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\left(\frac{\eta}{k}\mathbf{u}+\nabla p-\mathbf{F}\right)=0$$

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

where ρ denotes the density, η the viscosity, k the permeability, ε the porosity, $\mathbf{u}$ the velocity, p the pressure, and $\mathbf{F}$ a force term. 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 294 of the *Earth Science Module Model Library.*

Boundary Conditions

The predefined boundary conditions for the Brinkman Equation application mode follow. Inlet and outlet velocities at boundaries are

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

You can specify pressure as

$$p=p_0$$

Velocity that drops to zero at an impervious boundary corresponds to the no-slip condition

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

The normal flow, pressure condition sets the velocity to zero in the tangential direction, **t**, and it also specifies the outflow pressure in this way:

$$\mathbf{u} \cdot \mathbf{t} = 0$$
$$p = p_0$$

The neutral boundary condition neither constrains the flow nor gives rise to momentum transport; it simply states that transport by shear stress is zero across the boundary

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

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 ferofluids 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

$$\nabla \cdot \mathbf{u} = 0 \qquad (2\text{-}4)$$

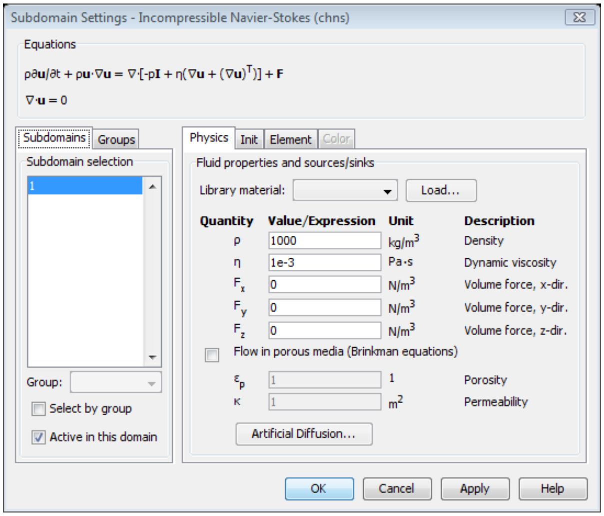
and the stress tensor τ becomes

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

These assumptions put together give the following momentum equations:

$$\rho\frac{\partial\mathbf{u}}{\partial t} + (\rho\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nabla\cdot(\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}})) + \mathbf{F} \qquad (2\text{-}5)$$

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 2-3).



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

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

Quantity	Value/Expression	Unit	Description
ρ	1000	kg/m^3	Density
η	1e-3	Pa·s	Dynamic viscosity
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.
ε_p	1	1	Porosity
κ	1	m^2	Permeability

Figure 2-3: 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

$$\mathrm{Re} = \frac{d u_0 \rho}{\eta}$$

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

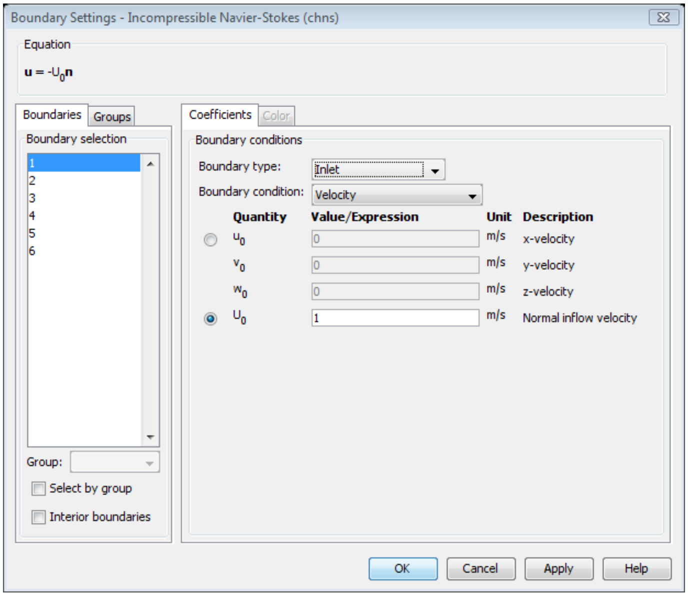
The Navier-Stokes application mode automatically calculates the cell Reynolds number using the element length h for d and the magnitude of the velocity vector U for u_0. Modeling turbulent flow with the Navier-Stokes equations requires a large number of nodes to resolve small eddies that can move through 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
- 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 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 2-4: 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. ?.

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

$$\mathbf{u} = \mathbf{u}_w$$

Note that setting this boundary condition does not automatically cause the associated wall to move. The section "The Moving Mesh Application Mode" on page 401 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 $\mathrm{U_w}$ and the condition prescribes

$$\mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{u} \cdot \mathbf{t} = \mathrm{U_w}$$

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:

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

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:

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

Note 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 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 1.

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:

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

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 1.

Observe 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 $\mathrm{Re}^c = \rho|\mathbf{u}|h/2\eta \gg 1$. It is far less stable than the Pressure, no viscous stress boundary condition, but it is consistent with a non-normal outflow velocity.

No Viscous Stress

Prescribes vanishing viscous stress:

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

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 1).

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:

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

This of course 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

$$p = 2\eta\frac{\partial u_n}{\partial n} + \mathrm{f}_0 \tag{2-6}$$

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

SYMMETRY BOUNDARY

Prescribes no penetration and vanishing shear stresses:

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

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:

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

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 1).

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:

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

This of course 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

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

If $\partial u_n/\partial n$ is small, Equation ?-??? 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 $\mathbf{F}$:

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

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

$$p = 2\eta\frac{\partial u_n}{\partial n} - \mathbf{n}\cdot\mathbf{F} \tag{2-8}$$

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

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

This of course 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

$$p = 2\eta\frac{\partial u_n}{\partial n} + \mathrm{f}_0 \tag{2-9}$$

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

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

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

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

If $\partial u_n/\partial n$ is small, Equation ?-??? 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—Artificial Diffusion

The momentum equations (Equation 5-7) are of convection-diffusion type. It is well known that if standard Galerkin discretization is used, such equations become unstable for an element Peclet number (Pe) larger than one (Ref. ?):

$$\mathrm{Pe} = \frac{\rho\|\mathbf{u}\|h}{2\eta} > 1 \tag{2-11}$$

where h is the element size. The instabilities might cause the simulation to diverge. If a solution where Pe is larger than one is obtained, it can often have spurious oscillations even if the exact solution is smooth. Figure ?-??? shows an example of such ocscillations.

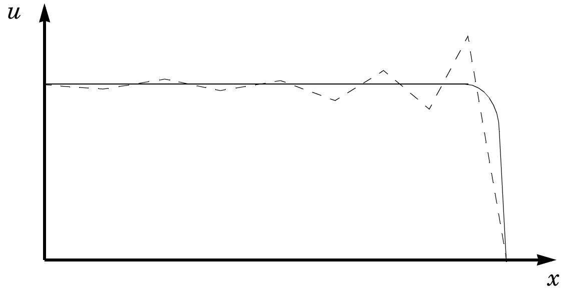
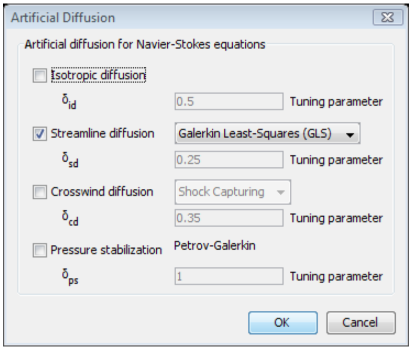


Figure 2-5: A 1D convection diffusion example with Pe > 1. *The exact solution (solid line) is smooth while the solution obtained by standard Galerkin discretization (dashed line) contains spurious oscillations.*

The element Peclet number can always be made less than one by refining the mesh, that is, by making the mesh element size h small enough. This method is not always feasible because it can require a very dense mesh. Instead, so-called stabilization methods, or artificial diffusion, are used. COMSOL Multiphysics provides several of these methods. The dialog box for selecting artificial diffusion (Figure ?-???) is opened from the **Subdomain Settings** dialog box by clicking the **Artificial Diffusion** button (see Figure 5-1 on page 109).



Artificial Diffusion

Artificial diffusion for Navier-Stokes equations

☐ Isotropic diffusion

δ_{id} 0.5 Tuning parameter

☑ Streamline diffusion Galerkin Least-Squares (GLS)

δ_{sd} 0.25 Tuning parameter

☐ Crosswind diffusion Shock Capturing

δ_{cd} 0.35 Tuning parameter

☐ Pressure stabilization Petrov-Galerkin

δ_{ps} 1 Tuning parameter

Figure 2-6: The Artificial Diffusion dialog box showing the default setting: Galerkin least-squares (GLS) streamline diffusion.

None of the artificial diffusion methods allows arbitrarily high Peclet numbers. As the Peclet number goes to infinity, they either lose their stabilizing effect or completely destroy the solution.

To use no artificial diffusion at all corresponds to the standard Galerkin discretization. A requirement for stability is then that higher-order basis functions must be used for the velocities than for the pressure. This condition is know as the Babuska-Brezzi condition or the inf-sup stability condition (Ref. ? and ?). Two of the artificial diffusion methods provided in COMSOL Multiphysics can relax the Babuska-Brezzi condition: Galerkin least-squares (GLS) and pressure stabilization.

The mathematical description of the methods is given in Chapter 15, “Stabilization Techniques,” in the *COMSOL Multiphysics Modeling Guide*.

ISOTROPIC DIFFUSION

Isotropic diffusion increases the viscosity in regions where the Peclet number is large. Hence, the original equation is perturbed. This method can force the simulation to be stable, but there is no guarantee that the solution is the correct physical solution.

STREAMLINE DIFFUSION

In most cases, spurious oscillations arise in the streamline direction only. Streamline diffusion methods introduce diffusion in the streamline direction by weighting the discretization scheme in the upstream direction. This means that more information is taken from the direction from which information is convected and less from the direction in which the information is traveling. Streamline-diffusion methods are closely related to the upwind methods in finite difference and finite volume methods.

Anisotropic Streamline Diffusion

This method projects the extra diffusion onto the streamlines and is therefore much less brutal than the isotropic diffusion. Still, the method is not consistent, meaning that the exact solution does not solve the discrete system. Therefore, the accuracy of the solution cannot be guaranteed.

Streamline Upwind Petrov-Galerkin (SUPG)

The Streamline Upwind Petrov-Galerkin method is a consistent method, which means that it does not perturb the equations. A model that converges with this method can be considered to be a solution to the discrete counterpart of Equation 5-6 and Equation 5-7. This method is somewhat less stabilizing than the anisotropic streamline diffusion because the terms that differ between the methods are mainly destabilizing.

Streamline Upwind Petrov-Galerkin (SUPG), Compensated

This version of SUPG turns off the diffusion in regions with element Peclet number less than one.

Galerkin Least-Squares (GLS)

The Galerkin least-squares (GLS) method is a consistent method that circumvents the Babuska-Brezzi condition, that is, it is possible to use equal-order elements for the velocities and the pressure.

For the momentum equations, GLS has many of its stability properties in common with SUPG. The superior stability of GLS can often be explained by the stabilizing terms on the continuum equation, terms that SUPG lacks.

GLS is activated per default even though it is more expensive to assemble than SUPG. The extra cost is often more than compensated for by the superior stability properties of GLS.

CROSSWIND DIFFUSION

In some cases, diffusion in the streamline direction is not enough to enforce stability. This is the situation in thin boundary layers and shear layers where there are large gradients in directions orthogonal to the streamline direction.

Ordo $h^{3/2}$

The Ordo $h^{3/2}$ method is an efficient and inexpensive method with good convergence properties. It is not consistent but has good accuracy compared to methods of similar complexity. However, the method is constructed exclusively for linear elements and it is dimensionally inconsistent. The latter is important to note if the model uses other units than SI units.

Shock Capturing

This method is more general and often better than the Ordo $h^{3/2}$ method. It is also consistent and independent of which units that are used. It is, however, considerably more computationally expensive than the Ordo $h^{3/2}$ method.

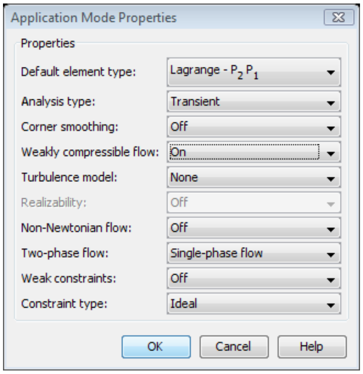
PRESSURE STABILIZATION

The main feature of this method is that it circumvents the Babuska-Brezzi condition. It can also add stability essential to iterative solvers.

Pressure stabilization together with SUPG can be regarded as a less expensive and less stable version of GLS. Pressure stabilization should not be used together with GLS.

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 2-7: The Application Mode Properties dialog box where Corner smoothing can be turned on and off.

Consider the situation sketched in Figure ?-???. At the point where the boundaries Γ_1 and Γ_2 intersect, there will be 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 ?-???. If the boundaries now both have no-penetration condition, there will be two Dirichlet conditions at the point of intersection, namely

$$\mathbf{n}_{\Gamma_1} \cdot \mathbf{u} = 0 \tag{2-12}$$

and

$$\mathbf{n}_{\Gamma_2} \cdot \mathbf{u} = 0 \tag{2-13}$$

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

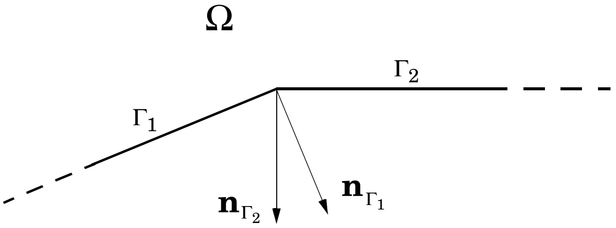


Figure 2-8: Intersection between the boundaries Γ_1 *and* Γ_2. $\mathbf{n}_{\Gamma_1}$ *and* $\mathbf{n}_{\Gamma_2}$ *are the boundary normals prescribed by* Γ_1 *and* Γ_2 *respectively.* Ω *is the computational domain.*

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 ?-??? and ?-??? are replaced with

$$\mathbf{n}_\mathrm{w} \cdot \mathbf{u} = \mathbf{0} \tag{2-14}$$

and $\mathbf{n}_\mathrm{w}$ has the solution $\mathbf{n}_\mathrm{w} = 1/2(\mathbf{n}_{\Gamma_1} + \mathbf{n}_{\Gamma_2})$. Equation ?-??? 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 tables (where x_i denotes the various space coordinate directions):

NAME	TYPE	DESCRIPTION	EXPRESSION
u, v, (w)	B S V	x_i velocity	u, v, w
p	B S	Pressure	p

NAME	TYPE	DESCRIPTION	EXPRESSION
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)
Vx*i*	S	Vorticity	x_i components of $\nabla \times \mathbf{u}$ (3D)
rho	S	Density	ρ
eta	S	Dynamic viscosity	η
F_x*i*	S	Volume force, x_i dir.	x_i components of $\mathbf{F}$
K_x*i*	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_x*i*	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_u*i*_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_u*i*_c	S	Shock capturing residual, u_i component	$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \mathbf{F}$ (u_i component)
beta_x*i*	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.)

General 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 497 in the *COMSOL Multiphysics Reference Guide*. The problem occurs when one solution component is identically zero.

Solver Settings

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 GMRES with the geometric multigrid (GMG) preconditioner. The GMG preconditioner uses the Vanka preconditioner/smoother as the presmoother and postsmoother.

For more information about the solvers, see Chapter 6, "Solving the Model," on page 359 in the *COMSOL Multiphysics User's Guide*.

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 497 in the *COMSOL Multiphysics Reference Guide*. The problem occurs when one solution component is close to 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. ?).

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

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

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

Thew 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 defined by clicking the **Parameters** button. Table 0-1 shows the default values for this parameter:

TABLE 2-2: PARAMETER FOR THE KHAN AND RICHARDSON FORCE

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

The particle mass appears in the force equation, and you enter its value in the **m** 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.

References

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

2. O.C. Zienkiewicz, R.L. Taylor, and P. Nithiarasu, *The Finite Element Method for Fluid Dynamics*, Sixth edition, Elsevier, 2005.

3. C. Johnson, *Numerical solution of partial differential equations by the finite element method*, Studentlitteratur, 1987.

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

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:

$$\begin{gathered}\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0\\ \rho\frac{\partial\mathbf{u}}{\partial t}+\rho\mathbf{u}\cdot\nabla\mathbf{u}=-\nabla p+\nabla\cdot\left(\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)-\left(\frac{2}{3}\eta-\kappa_{\mathrm{dv}}\right)(\nabla\cdot\mathbf{u})\mathbf{I}\right)+\mathbf{F}\end{gathered}\qquad(2\text{-}15)$$

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)

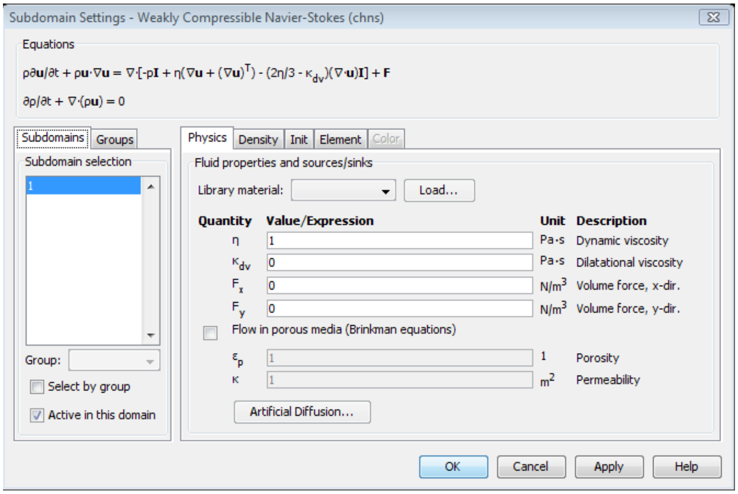
The stress tensor used in Equation 2-15 describes a Newtonian fluid but with an extra term κ_{dv}. This term expresses the deviation from Stokes' assumption, which states that the fluid particles are in thermodynamic equilibrium with their neighbors. It is very rare that a fluid shows a significant deviation from Stokes' assumption, and κ_{dv} is therefore by default set to zero.

SUBDOMAIN SETTINGS

The **Subdomain Settings** dialog box is shown in Figure 2-9. Unlike the Incompressible Navier-Stokes application mode, the edit field for the density, ρ, is not on the **Physics** page. Instead, it has its own page labeled **Density**. The content of the **Density** page is shown in Figure 2-10 on page 50. In addition to the edit field for the density, ρ, there are two check boxes. These are used to control the exact weak expression for the

Galerkin least-squares (GLS) artificial diffusion. This method, described in Chapter 15, “Stabilization Techniques,” of the *COMSOL Multiphysics Modeling Guide*, is necessary to get a stable finite element discretization of the equation system 2-15. You can define the density as a function of any of the other dependent variables, but GLS can only stabilize with respect to pressure and temperature, which are the most common variables.

Typically, the Weakly Compressible Navier-Stokes application mode is coupled to a heat equation that describes the variations in the temperature field.



Subdomain Settings - Weakly Compressible Navier-Stokes (chns)

Equations

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

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

Subdomain selection: 1

Group:

☐ Select by group

☑ Active in this domain

Fluid properties and sources/sinks

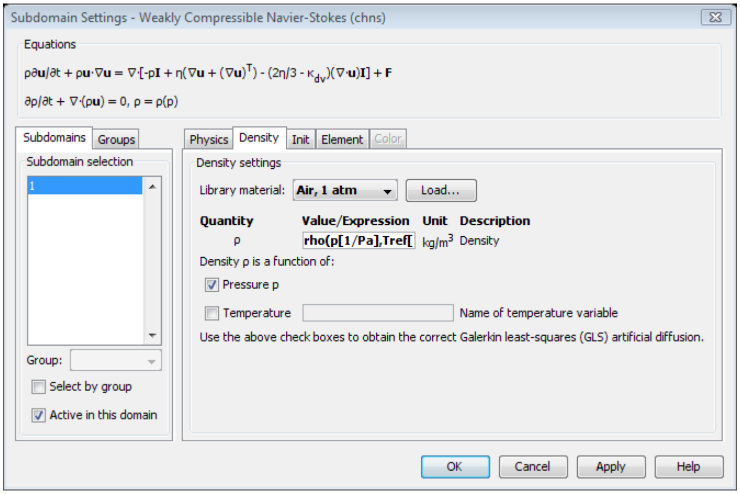
Library material:

Quantity	Value/Expression	Unit	Description
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)

Quantity	Value/Expression	Unit	Description
ϵ_p	1	1	Porosity
κ	1	m^2	Permeability

Figure 2-9: The Subdomain Settings dialog box for the Weakly Compressible Navier-Stokes application mode. Physics page.



Subdomain Settings - Weakly Compressible Navier-Stokes (chns)

Equations

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

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

Subdomain selection: 1

Group:

☐ Select by group

☑ Active in this domain

Density settings

Library material: **Air, 1 atm**

Quantity	**Value/Expression**	**Unit**	**Description**
ρ	**rho(p[1/Pa],Tref[**	kg/m^3	Density

Density ρ is a function of:

☑ Pressure p

☐ Temperature ☐ Name of temperature variable

Use the above check boxes to obtain the correct Galerkin least-squares (GLS) artificial diffusion.

Figure 2-10: The Subdomain Settings dialog box for the Weakly Compressible Navier-Stokes application mode. The Density page.

The Non-Isothermal Flow description of the Navier-Stokes equations can be used to describe free convection due to changes in density. In such a case, set the volume force term, **F**, to the gravity force, ρ**g**, where **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 2-4 and Equation 2-5 can be written

$$\frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{\partial u_z}{\partial z} = 0 \qquad (2\text{-}16)$$

$$\begin{aligned}
\rho\left(\frac{\partial u_r}{\partial t} + u_r\frac{\partial u_r}{\partial r} + u_z\frac{\partial u_r}{\partial z} - \frac{u_\varphi^2}{r}\right) &= -\frac{\partial p}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rr}) + \frac{\partial \tau_{zr}}{\partial z} - \frac{\tau_{\varphi\varphi}}{r} + F_r \\
\rho\left(\frac{\partial u_z}{\partial t} + u_r\frac{\partial u_z}{\partial r} + u_z\frac{\partial u_z}{\partial z}\right) &= -\frac{\partial p}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rz}) + \frac{\partial \tau_{zz}}{\partial z} + F_z \\
\rho\left(\frac{\partial u_\varphi}{\partial t} + u_r\frac{\partial u_\varphi}{\partial r} + \frac{u_r u_\varphi}{r} + u_r\frac{\partial u_\varphi}{\partial z}\right) &= \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\tau_{r\varphi}) + \frac{\partial \tau_{z\varphi}}{\partial z} + F_\varphi
\end{aligned} \qquad (2\text{-}17)$$

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 2-11.

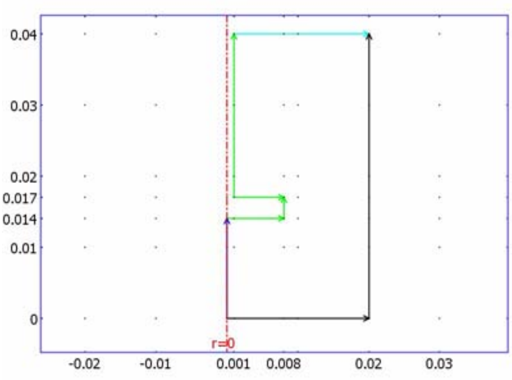


Figure 2-11: A geometry drawn in the 2D Axial Symmetry space dimension. Notice that the whole domain must be contained to the right of the symmetry line $r = 0$.

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 39, and “Numerical Stability—Artificial Diffusion” 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.

Solute Transport Application Mode

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:

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

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).

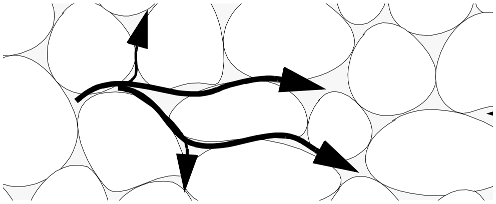
The retardation factor, RF, describes how sorption slows the solute velocity, $\mathbf{u}_c$, relative to the average linear velocity of the fluid, $\mathbf{u}_a$, as in

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

If the contaminant moves at the average linear velocity of the fluid for $\mathrm{RF} = 1$. For $\mathrm{RF} > 1$, 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 $\alpha_{3,}$ 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 $\tau_L = \theta^{7/3}\,\theta_s^{-2}$ 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

$R_{Li} = -\theta_s \frac{\ln 2}{\lambda_{Li}} c_i$	Radioactive decay—liquid
$R_{Pi} = -\rho_b \frac{\ln 2}{\lambda_{Pi}} \left(\frac{\partial c_{Pi}}{\partial c_i}\right) c_i$	Radioactive decay—solid
$R_{Lk} = \theta_s \zeta_{Li} c_i$	Creation from parent c_{Li} —liquid
$R_{Pk} = \rho_b \zeta_{Pi} \left(\frac{\partial c_{Pi}}{\partial c_i}\right) c_i$	Creation from sorbed parent c_{Pi} —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_{Pi} 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:

$$\zeta_T = \zeta_R \exp\left[\frac{E_a(T - T_R)}{R_u T T_R}\right]$$

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 that states both the concentration and the boundary flux. The final 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.

$$\begin{array}{ll}
c_i = c_{i,\,0} & \text{Concentration} \\
\mathbf{n}\cdot(\theta_s D_{Li}\nabla c_i - \mathbf{u}c_i) = N_{i,\,0} & \text{Flux} \\
\mathbf{n}\cdot(\theta_s D_{Li}\nabla c_i - \mathbf{u}c_i) = 0 & \text{No flux} \\
\mathbf{n}\cdot(\theta_s D_{Li}\nabla c_i - \mathbf{u}c_i) = \mathbf{n}\cdot\mathbf{u}c_{i,\,0} + N_{i,\,0} & \text{General} \\
\mathbf{n}\cdot(\theta_s D_{Li}\nabla c_i) = 0 & \text{Advective flux}
\end{array}$$

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

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

suits compressible fluids, in which density varies spatially.

The nonconservative form

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

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

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

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:

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_b c_P) + \frac{\partial}{\partial t}(a_v c_G) = \theta\frac{\partial c}{\partial t} + \rho_b k_p \frac{\partial c}{\partial t} + a_v k_G \frac{\partial c}{\partial t} + (1 - k_G) c \frac{\partial \theta}{\partial t}$$

Here, the liquid-to-solid and liquid-to-gas partitioning are governed by the sorption isotherm $k_P = \partial c_P / \partial c$ and volatilization isotherm $k_G = \partial c_G / \partial c$. The air volume, a_v, is the empty portion of the total porosity θ_s, so it varies as the liquid volume fraction changes $a_v = \theta_s - \theta$.

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 54. 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 $\mathbf{u}_a$ is given by:

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

where the specific velocity describes the net value over surface made up of liquid, solid, and gas $\mathbf{u}$. 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:

$$\begin{array}{lll l} c_P = Kc & \dfrac{\partial c_P}{\partial c} = K & & \text{Linear} \\ c_P = K_F c^N & \dfrac{\partial c_P}{\partial c} = NK_F c^{N-1} & & \text{Freundlich} \\ c_P = \dfrac{K_L \bar{s} c}{1 + K_L c} & \dfrac{\partial c_P}{\partial c} = \dfrac{K_L \bar{s}}{1 + K_L c^2} & & \text{Langmuir} \end{array}$$

In these equations, the partial derivatives describe the relationship between c_i and c_{Pi} at equilibrium. In COMSOL Multiphysics you also can enter arbitrary expression 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, $\mathbf{u}_a$, which now varies with the liquid content. The retardation factor, RF becomes:

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

As discussed for saturated solute transport, the contaminant moves at the average linear velocity of the fluid for $RF = 1$. For $RF > 1$, 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:

$$\theta D_{LGii} = \alpha_1 \frac{u_i^2}{|\mathbf{u}|} + \alpha_2 \frac{u_j^2}{|\mathbf{u}|} + \theta D_m \tau_L + a_v D_G k_G \tau_G$$

$$\theta D_{LGij} = \theta D_{LGji} = (\alpha_1 - \alpha_2)\frac{u_i u_j}{|\mathbf{u}|}.$$

In these equation, D_{LGii} are the principal components of the liquid-gas dispersion tensor; D_{LGji} and D_{LGji} 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 provides options to define $\tau_L = \theta^{7/3}\,\theta_s^{-2}$ and $\tau_G = a_v^{\,7/3}\,\theta_s^{-2}$ or enter arbitrary expressions.

Reactions

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

$$\begin{aligned} R_G &= -\frac{\ln 2}{\lambda_{Gi}} a_v\left(\frac{\partial c_G}{\partial c}\right)c && \text{Radioactive decay—gas} \\ R_G &= -\zeta a_v\left(\frac{\partial c_G}{\partial c}\right)c && \text{Reaction—gas} \end{aligned}.$$

where λ is the chemical half life, 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,

$$\begin{aligned} R_L &= -\theta\frac{\ln 2}{\lambda_{Li}} c_i && \text{Radioactive decay—liquid} \\ R_L &= -\theta\zeta_L c_i && \text{Reaction—liquid} \end{aligned}.$$

Boundary Conditions

In variably saturated porous media new boundary conditions describe interactions with adjacent gas phases. You can use the no flow boundary volatilization option 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:

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

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 condition:

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

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
$\mathbf{n}\cdot(\theta D_{LG}\nabla c - \mathbf{u}c) = N_0$	Flux
$\mathbf{n}\cdot(\theta D_{LG}\nabla c - \mathbf{u}c) = 0$	No flux
$\mathbf{n}\cdot(\theta D_{LG}\nabla c - \mathbf{u}c) = \mathbf{n}\cdot\mathbf{u}c_0 + N_0$	General
$\mathbf{n}\cdot(\theta D_{LG}\nabla c) = 0$	Advective flux

Conservative and Non-Conservative 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

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

suits compressible fluids, in which density varies spatially.

The nonconservative form

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

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

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Heat Transfer Application Modes

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.

Heat Transfer—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

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

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, $\mathbf{N}$, 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

$$C_{\mathrm{eq}} = \frac{\Sigma\theta_{Li}\rho_{Li}C_{pLi} + \Sigma\theta_{Pi}\rho_{Pi}C_{pPi}}{\Sigma\theta_{Li} + \Sigma\theta_{Pi}}$$

$$K_{\mathrm{eq}} = \frac{\Sigma\theta_{Li}K_{Li} + \Sigma\theta_{Pi}K_{Pi}}{\Sigma\theta_{Li} + \Sigma\theta_{Pi}}$$

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.

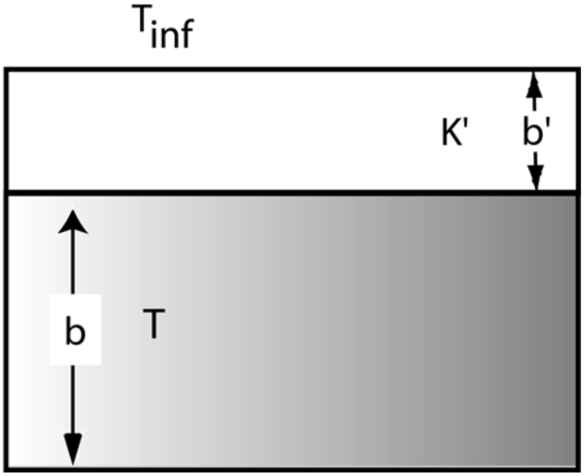
You can describe sensible heat transfer from the soil to some air flowing over the domain as

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

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

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

Here the model sets T_{ref} to 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

$$\delta_{\mathrm{ts}} C_{\mathrm{eq}} \frac{\partial T}{\partial t} + \nabla \cdot [-K_{\mathrm{eq}} \nabla T + C_L \mathbf{u} T] = Q_H + Q_G \,. \tag{2-18}$$

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

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

where **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 "Heat Transfer–Conduction" on page 69.

Boundary Conditions

The Convection and Conduction 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 boundary conditions are

$T = T_0$		Temperature
$T = 0$		Zero temperature
$-\mathbf{n} \cdot N = N_0,$	$N = -K_{\mathrm{eq}}\nabla T + C_L \mathbf{u} T$	Heat flux
$-\mathbf{n} \cdot N = 0,$	$N = -K_{\mathrm{eq}}\nabla T$	Convective flux
$-\mathbf{n} \cdot N = 0,$	$N = 0$	Thermal insulation
$-\mathbf{n} \cdot N = 0,$	$N = 0$	Axial symmetry.

In these equations, T_0 and N_0 are the temperatures and the fluxes that you define, and $\mathbf{n}$ is the normal vector to the boundary.

The fundamental piece of data in many environmental scenarios is a measurement of temperature, a Dirichlet condition. You can enter the boundary temperature as a constant, model results, or as a string of data and allow the software to interpolate 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 Dirichlet 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 $\bar{T}$ 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.

Conservative and Nonconservative Formulations

For incompressible fluids and other cases where you can assume that the divergence in the velocity is zero, it is possible to restate the governing equation in the following nonconservative form:

$$\delta_{\mathrm{ts}}\ C_{\mathrm{eq}}\frac{\partial T}{\partial t} + \nabla \cdot (-K_{\mathrm{eq}}\nabla T) \ = -C_L\mathbf{u}\nabla T + Q_H + Q_G\,. \tag{2-19}$$

Both the conservative form in Equation 2-18 and the nonconservative form in Equation 2-19 are options in the application mode.

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

$$C_{\mathrm{eq}} = \frac{\theta_L \rho_L C_{pL} + \Sigma\theta_{Gi}\rho_{Gi}C_{pGi} + \Sigma\theta_{Pi}\rho_{Pi}C_{pPi}}{\theta_L + \Sigma\theta_{Gi} + \Sigma\theta_{Pi}}$$

$$C_L = \rho_L \dot{C}_{pL}$$

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

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

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

$$\begin{aligned}
K_{\mathrm{Disp}xx} &= \lambda_1 C_L \frac{u^2}{|\mathbf{u}|} + \lambda_2 C_L \frac{v^2}{|\mathbf{u}|} + \lambda_3 C_L \frac{w^2}{|\mathbf{u}|} \\
K_{\mathrm{Disp}yy} &= \lambda_1 C_L \frac{v^2}{|\mathbf{u}|} + \lambda_2 C_L \frac{u^2}{|\mathbf{u}|} + \lambda_3 C_L \frac{w^2}{|\mathbf{u}|} \\
K_{\mathrm{Disp}zz} &= \lambda_1 C_L \frac{w^2}{|\mathbf{u}|} + \lambda_3 C_L \frac{u^2}{|\mathbf{u}|} + \lambda_3 C_L \frac{v^2}{|\mathbf{u}|} \\
K_{\mathrm{Disp}xy} &= K_{\mathrm{Disp}yx} = (\lambda_1 - \lambda_2) C_L \frac{uv}{|\mathbf{u}|} \\
K_{\mathrm{Disp}xz} &= K_{\mathrm{Disp}zx} = (\lambda_1 - \lambda_3) C_L \frac{uw}{|\mathbf{u}|} \\
K_{\mathrm{Disp}yz} &= K_{\mathrm{Disp}zy} = (\lambda_1 - \lambda_3) C_L \frac{vw}{|\mathbf{u}|}
\end{aligned}$$

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

$$K_{\mathrm{eq}} = K_{\mathrm{PM}} = \frac{\theta_L K_L + \Sigma\theta_{Gi} K_{Gi} + \Sigma\theta_{Pi} K_{Pi}}{\theta_L + \Sigma\theta_{Gi} + \Sigma\theta_{Pi}} .$$

Artificial Diffusion

Modeling transport phenomena for complex geometries usually requires numerical solutions based on some kind of discretization, and in COMSOL Multiphysics' case in the form of finite elements. The discretization of convection-dominated transport problems can introduce instabilities in the solution. The Convection and Conduction application mode supports the artificial diffusion stabilization technique. For information about this technique, see "Stabilization Techniques" on page 433 in the *COMSOL Multiphysics Modeling Guide*.

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.

3. G. de Marsily, *Quantitative Hydrogeology*, Academic Press, 1986.

3

Application Modes Reference

This section 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.

To facilitate quick reference, the application modes are listed alphabetically.

Definition of the Application Modes

Module Setup

The Model Navigator tree control for the Earth Science Module is structured as follows:

Fluid Flow

- Incompressible Navier-Stokes
    - **a** Steady-state
    - **b** Steady-state with multigrid
    - **c** Transient
- Brinkman Equations
    - **a** Steady-state
    - **b** Transient
- Darcy's Law
    - **a** Pressure analysis
    - **-** Steady-state
    - **-** Transient
    - **b** Pressure head analysis
    - **-** Steady-state
    - **-** Transient
    - **c** Hydraulic head analysis
    - **-** Steady-state
    - **-** Transient

- Richards' Equation
  - **a** Pressure analysis
    - Steady-state
    - Transient
  - **b** Pressure head analysis
    - Steady-state
    - Transient
  - **c** Hydraulic head analysis
    - Steady-state
    - Transient

Solute Transport

- Saturated Porous Media
  - **a** Steady-state
  - **b** Transient
- Variably Saturated Porous Media
  - **a** Steady-state
  - **b** Transient

Heat Transfer

- Conduction
  - **a** Steady-state
  - **b** Transient
- Convection and Conduction
  - **a** Steady-state
  - **b** Transient

All of the application modes are available in Cartesian (x, y) and cylindrical (r, z) coordinates with rotational symmetry or axisymmetry. The symmetry line in the axisymmetrical application modes is the z-axis. The geometry must lie in the half plane $r > 0$. The Navier-Stokes equations and the Brinkman equations are not available in 1D because the equations require physics in multiple dimensions.

Definition of the Equations in COMSOL Multiphysics

The following section details 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 variable and application mode variables in expressions and postprocessing. Following are the different **Application Mode Properties** you can trigger (such as non-isothermal flow or pressure head analysis). 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
axisymmetry 1D	r		
axisymmetry 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 used for modeling free flows, typically in the absence of porous media such as in rivers, caverns, pipes, 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 given in the table below.

TABLE 3-1: 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 3-1: 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 3-1 on page 88.

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 $\kappa = A_r\ \kappa_s$ 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 contains interfaces for: (1) **Coefficients**, (2) **Scaling Terms**, (3) **Init**, and (4) **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	
χ_f	chif	Compressibility of fluid	
χ_p	chip	Compressibility of solid	

SYMBOL	VARIABLE	DESCRIPTION	OPTIONS
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	

SCALING

The **Scaling** tab provides optional coefficients that you can use to scale different terms in your model. The scaling terms 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	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_\mathrm{f}gD)\right] = N_0$	Inward flux
Nz	$\mathbf{n}\cdot\left[\frac{\kappa}{\eta}\nabla(p+\rho_f gD)\right] = 0$	Zero flux/Symmetry
Nm	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_\mathrm{f}gD)\right]$ $= N_0 + R_b[(p_b - p) + \rho_\mathrm{f}g(D_b - D)]$	Mixed
Na	$\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_\mathrm{f}gD)\right] = 0$	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	$-\mathbf{n} \cdot (-K\nabla H)$ $= N_0 + R_b(H_b - H)$	$-\mathbf{n} \cdot [-\underline{K}\nabla(H_p + D)]$ $= N_0 + R_b[(H_{pb} - H_p) + (D_b - D)]$	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
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

The following equation coefficients are available to use in terms and expressions. You access them using 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 3-2: APPLICATION MODE VARIABLES, DARCY'S LAW.

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}
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)

TABLE 3-2: APPLICATION MODE VARIABLES, DARCY'S LAW.

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
Qs	All	B/S	Fluid sources	$Q_s\delta_{Qs}$
K	All	B/S/E/P	Hydraulic conductivity tensor	$K_s\delta K_s$
Kx`i`x`j`	All	B/S/E/P	Hydraulic conductivity tensor, x_ix_j component	K_{ij}
kap	All	B/S/E/P	Permeability tensor	$\kappa_s\delta_{Ks}$
kapx`i`x`j`	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	$\lvert\nabla p\rvert$
px`i`	All	V	Pressure gradient, x_i component	$\frac{\partial p}{\partial x_i}$
Hp	Hp	B/S/E/P	Pressure head	$p/(\rho_{\mathrm{f}}g)$
gradHp	Hp	B/S/E/P	Pressure head gradient, norm	$\lvert\nabla H_p\rvert$
Hpx`i`	Hp	V	Pressure head gradient, x_i component	$\frac{\partial H_p}{\partial x_i}$
H	H	B/S/E/P	Hydraulic head	$p/(\rho_{\mathrm{f}}g)+D$
gradH	H	B/S/E/P	Hydraulic head gradient, norm	$\lvert\nabla(H)\rvert$
Hx`i`	H	V	Hydraulic head gradient, x_i component	$\frac{\partial H}{\partial x_i}$
u,v,w	All	V	Darcy velocity x_i	$-\frac{\kappa}{\eta}\frac{\partial}{\partial x_i}(p+\rho_{\mathrm{f}}gD)$ (permeability) $-\frac{K}{\rho_{\mathrm{f}}g}\frac{\partial}{\partial x_i}(p+\rho_{\mathrm{f}}gD)$ (conductivity)
U	All	B/S/E/P	Total Darcy velocity	$\sqrt{u^2+v^2+w^2}$

TABLE 3-2: APPLICATION MODE VARIABLES, DARCY'S LAW.

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
nU	All	B	Normal Darcy velocity	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_\mathrm{f}gD)\right]$ (permeability) $-\mathbf{n}\cdot\left[-\frac{K}{\rho_\mathrm{f}g}\nabla(p+\rho_\mathrm{f}gD)\right]$ (conductivity)
flux	All	B	Boundary flux	$-\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p+\rho_\mathrm{f}gD)\right]$ (permeability) $-\mathbf{n}\cdot\left[-\frac{K}{\rho_\mathrm{f}g}\nabla(p+\rho_\mathrm{f}gD)\right]$ (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

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

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 may also be solved in terms of hydraulic conductivity by substituting the following:

$$\frac{\kappa}{\eta} = A_r\frac{K_sk_r}{\rho_fg} = A_r\frac{\kappa_sk_r}{\eta}$$

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.

$$H_p = H - D = \frac{p}{\rho_{\mathrm{f}} g_r}$$

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

$$S_s = [\chi_p(1 - \theta_s) + \chi_p \theta_s] \qquad C = C(H_p)/(\rho_{\mathrm{f}} g)$$

The definitions for analysis type H read

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

For H_p the definitions are

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

Subdomain Settings

The following tables give the parameters and equation coefficients for subdomain settings dialogs. Included are the tabs: (1) **Coefficients**, (2) **Van Genuchten**, (3) **Brooks & Corey**, (4) **User Defined**, (5) **Init**, (6) **Element**.

COEFFICIENTS

The **Coefficients** tab 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** tabs provide expression fields for:

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

When the **Van Genuchten** tab is active the retention and permeability relationships are defined according to:

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

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

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

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

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

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

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

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

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

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

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	$p = 0$	Water table/Seepage face
N0	$-\mathbf{n} \cdot \left[-\frac{\kappa}{\eta} k_r \nabla(p + \rho_f g D)\right] = N_0$	Inward flux
Nz	$\mathbf{n} \cdot \left[\frac{\kappa}{\eta} k_r \nabla(p + \rho_f g D)\right] = 0$	Zero flux/Symmetry
Nm	$-\mathbf{n} \cdot \left[-\frac{\kappa}{\eta} k_r \nabla(p + \rho_f g D)\right]$ $= N_0 + R_b[(p_b - p) + \rho_f g(D_b - D)]$	Mixed
Na	$\mathbf{n} \cdot \left[-\frac{\kappa}{\eta} k_r \nabla(p + \rho_f g D)\right] = 0$	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	$H = D$	$H_p = 0$	Water table/Seepage face
N0	$-\mathbf{n} \cdot (-K k_r \nabla H) = N_0$	$-\mathbf{n} \cdot [-K k_r \nabla(H_p + D)] = N_0$	Inward flux
Nz	$\mathbf{n} \cdot (K k_r \nabla H) = 0$	$\mathbf{n} \cdot [K k_r \nabla(H_p + D)] = 0$	Zero flux/Symmetry
Nm	$-\mathbf{n} \cdot (-K k_r \nabla H)$ $= N_0 + R_b(H_b - H)$	$-\mathbf{n} \cdot [-K k_r \nabla(H_p + D)]$ $= N_0 + R_b[(H_{pb} - H_p) + (D_b - D)]$	Mixed
Na	$\mathbf{n} \cdot (-K k_r \nabla H) = 0$	$\mathbf{n} \cdot [-K k_r \nabla(H_p + D)] = 0$	Axial symmetry

Point Settings, Edge Settings, 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 and are not repeated here.

Application Mode Variables

The application mode variables are predefined quantities and are given in the following tables for equation coefficients, retention and permeability relationships, and other application mode variables including gradients and fluxes.

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

TABLE 3-3: APPLICATION MODE VARIABLES, RICHARDS' EQUATION.

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	$\frac{C_{vG}}{\rho_f g}$ (van Genuchten) $\frac{C_{BC}}{\rho_f g}$ (Brooks and Corey) $\frac{C_i}{\rho_{\mathrm{head}} g}$ (user defined)
Se	All	S/B/E/P		Se_{vG} (van Genuchten) Se_{BC} (Brooks and Corey) Se_i (user defined)
S	p	S/B/E/P	Storage term	$\chi_p(1-\theta_s)+\chi_f\theta_s$ (specific storage) S_i (user defined)

TABLE 3-3: APPLICATION MODE VARIABLES, RICHARDS' EQUATION.

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
S	Hp	S/B/E/P	Storage term	$\chi_p(1-\theta_s)+\chi_f\theta_s$ (specific storage) $\frac{S_i}{\rho_f g}$ (user defined)
p	p	S/B/E/P	Pressure	p
kaponeta	p	S/B/E/P	Permeability on viscosity	$\frac{\kappa}{\eta} = \frac{K}{\rho_f g_r}$
K	All	S/B/E/P	Hydraulic conductivity tensor	$K_s \kappa_r$
kap	All	S/B/E/P	Permeability tensor	$\kappa_s k_r$
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
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	$1-\frac{1}{n}$

TABLE 3-3: APPLICATION MODE VARIABLES, RICHARDS' EQUATION.

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
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) $\begin{array}{ll} (\theta_r + (\theta_s - \theta_r)Se) & \left(H_p < -\frac{1}{\alpha}\right) \\ \theta_s & \left(H_p \ge -\frac{1}{\alpha}\right) \end{array}$ (Brooks and Corey) $\begin{array}{l} \theta_i\ (H_p < \alpha) \\ \theta_s\ (H_p \ge \alpha) \end{array}$ (user defined)
C	All	S/B/E/P	Specific moisture capacity	$\begin{array}{ll} \frac{\alpha m}{1-m}(\theta_s - \theta_r)\mathrm{Se}^{\frac{1}{m}}\left(1 - \mathrm{Se}^{\frac{1}{m}}\right)^m & (H_p < 0) \\ 0 & (H_p \ge 0) \end{array}$ (van Genuchten) $\begin{array}{ll} -\frac{n}{H_p}(\theta_s - \theta_r)(\alpha H_p)^{-n} & \left(H_p < -\frac{1}{\alpha}\right) \\ 0 & \left(H_p \ge -\frac{1}{\alpha}\right) \end{array}$ (Brooks and Corey) $\begin{array}{l} C_i\ (H_p < \alpha) \\ 0\ \ (H_p \ge \alpha) \end{array}$ (user defined)

TABLE 3-3: APPLICATION MODE VARIABLES, RICHARDS' EQUATION.

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
Se	All	S/B/E/P	Effective saturation	$(1+(\alpha H_p)^n)^{-m} \quad (H_p < 0)$ $1 \quad (H_p \geq 0)$ (van Genuchten) $\alpha H_p{}^{-n} \quad \left(H_p < -\frac{1}{\alpha}\right)$ $1 \quad \left(H_p \geq -\frac{1}{\alpha}\right)$ (Brooks and Corey) $\mathrm{Se}_i \ (H_p < \alpha)$ $1 \quad (H_p \geq \alpha)$ (user defined)
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) $k_{ri} \ (H_p < \alpha)$ $1 \quad (H_p \geq \alpha)$ (user defined)
gradp	All	B/S/E/P	Pressure gradient, norm	$\lvert\nabla p\rvert$
px_i	All	V	Pressure gradient, x_i component	$\frac{\partial p}{\partial x_i}$

TABLE 3-3: APPLICATION MODE VARIABLES, RICHARDS' EQUATION.

NAME	ANALYSIS	TYPE	DESCRIPTION	EXPRESSION
gradHp	Hp	B/S/E/P	Pressure head gradient, norm	$\lvert\nabla H_p\rvert$
Hpx_i	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	$\lvert\nabla(H)\rvert$
Hx_i	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	$-\frac{\kappa}{\eta}\frac{\partial}{\partial x_i}(p+\rho_f g_r D)$
U	All	S/B/E/P	Total Darcy velocity	$\sqrt{u^2+v^2+w^2}$
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:

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

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** dialogs 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 Conditions

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 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_{Tf}	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_{Nf}	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

The following expressions and are available in equations and for postprocessing. Definitions for some variables depends on the analyses type and user options. In the Analysis column, S stands for Solid and PM for Porous Media.

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	Keqx_ix_j	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)
S,PM	QC	S	Convective heat source	$h_{\mathrm{trans}}(T_{\mathrm{ext}}-T)$

ANALYSIS	NAME	TYPE	DESCRIPTION	EXPRESSION
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	Tx_i	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	fluxx_i	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)	$\Sigma(\theta_{Pi}\rho_{Pi}Cp_{Pi})/\Sigma\theta_{Pi}$
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 is offered in conservative and non-conservative forms. Using the non-conservative form assumes the divergence in the velocity vector is zero. This formulation, which is the default in this application mode, reads:

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

With the conservative form, the fluid velocity appears inside the divergence operator:

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

Application Mode Properties

The **Application Mode Properties** dialog box available in the **Physics** menu or from the **Model Navigator** provides a menu to choose between the **conservative** and

non-conservative formulations. Another menu 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 contain interfaces for the following options: (1) **Materials**, (2) **Time/Convection**, (3) **Spreading**, (4) **Sources/Sinks**, (5) **Init**, and (6) **Element**.

MATERIALS

The **Materials** tab 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	Velocities in x_i direction	

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
$\lambda_{1,}$ $\lambda_{2,}$ λ_3	lambda1, lambda2, lambda3	Thermal dispersivity, x_1 direction
K_{PM}	KPM	Thermal conductivity, Porous Medium
$A_{r\mathrm{PM}}$	ArPM	Anisotropy ratio, Therm Cond PM Tensor

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

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

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:

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

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	$(\lambda_1 - \lambda_3)C_L vw/U$
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	$(\lambda_1 - \lambda_2)C_L uv/U$

SYMBOL	VARIABLE	DEFINITION
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** tab 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 Conditions

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

TYPE	BOUNDARY CONDITION	DESCRIPTION
T	$T = T_0$	Temperature
T0	$T = 0$	Zero 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 relevant coordinate systems. Also, for axisymmetric coordinate systems the q and g terms are multiplied by a factor r.

Point Settings, Edge Settings, Scalar Variables

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

Application Mode Variables

The application mode variables for Heat Transfer by Convection and Conduction are given in the following table. In the Analysis column MF stands for Mobile fluid, MF/S for Mobile fluid, solid and MF/IF/S for Mobile/immobile fluid, solid.

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)	$C_{eq} = C_L$
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) $K_{Disp} + K_{PM}$ (disp. and cond.) (or user entry)

ANALYSIS	Name	TYPE	DESCRIPTION	EXPRESSION
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) $K_{Disp}+K_{PM}$ (disp. and cond.) (or user entry)
All	Keqx_ix_j	S/B/E/P	Thermal conductivity (equivalent)	A_rK_{eq}
MF	Keq	S/B/E/P	Thermal conductivity (equivalent)	K_L
MF/S	KPM	S/B/E/P	Thermal conductivity (porous media)	$\frac{(\theta_LK_L+\theta_PK_P)}{\theta_L+\theta_P}$ (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)	$\rho_{geo}q_{geo}$ (uniform heat prod.) $\rho_{geo}q_{geo}h_{geo}\exp(z_{geo}/h_{geo})$ (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	Tx_i	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	$\lvert -K_{eq}\nabla T+C_L\mathbf{u}T\rvert$
MF/S, MF/IF/S	tfluxx_i	V	Total heat flux, x_i component	$(-K_{\mathrm{eq}}\nabla T+C_L\mathbf{u}T)_i$

ANALYSIS	Name	TYPE	DESCRIPTION	EXPRESSION
MF	tflux	S/B/E/P	Total heat flux, norm	$\lvert K_{\mathrm{eq}}\nabla T\rvert$
MF	tfluxx_i	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	dtfluxx_i	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	$\lvert K_{\mathrm{Disp}}\nabla T\rvert$
MF/S, MF/IF/S	difluxx_i	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	dfluxx_i	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	cfluxx_i	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

ANALYSIS	Name	**TYPE**	**DESCRIPTION**	**EXPRESSION**
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)	$\Sigma(\theta_{Gi}\rho_{Gi}Cp_{Gi})/\Sigma\theta_{Gi}$
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)	$\Sigma(\theta_{Pi}\rho_{Pi}Cp_{Pi})/\Sigma\theta_{Pi}$
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	$\lambda_1, \lambda_2, \lambda_3$
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	$\left\lvert\frac{\mathbf{u}h}{K_{\mathrm{eq}}}\right\rvert$
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, …, c_n.

PDE Formulation

The governing equation for saturated media is as follows:

$$\begin{aligned}&\delta_{\mathrm{ts1}}\left(\theta + \rho_b\frac{\partial c_{Pi}}{\partial c} + a_v\frac{\partial c_{Gi}}{\partial c}\right)\frac{\partial c}{\partial t} + \delta_{\mathrm{ts2}}(1-k_G)c\frac{\partial \theta}{\partial t}\\ &\text{" "} + \nabla\cdot[-\theta \mathrm{D}_{LGi}\nabla c_i + \mathbf{u}c_i] = R_{Li} + R_{Pi} + R_{Gi} + S_{ci}\end{aligned}$$

Here, c_i, $c_{Pi,}$ and c_{Gi}, respectively 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. In the equation, θ_s termed porosity is the volume of fluids divided by the total fluid-solid volume, $\rho_b = (1 - \theta_s)\rho_p$ is the bulk density of the porous medium when ρ_p is the particle density. D_{LGi} represents the hydrodynamic and gas dispersion tensor, and $\mathbf{u}$ is the vector of directional velocities. R_{Li}, R_{Pi} and R_{Gi} describe reactions in the liquid, solid and gas phases, 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 non-conservative form can be derived.

$$\begin{aligned}&\delta_{\mathrm{ts1}}\left(\theta + \rho_b\frac{\partial c_{Pi}}{\partial c} + a_v\frac{\partial c_{Gi}}{\partial c}\right)\frac{\partial c}{\partial t} + \delta_{\mathrm{ts2}}(1-k_G)c\frac{\partial \theta}{\partial t}\\ &\text{" "} + \nabla\cdot[-\theta \mathrm{D}_{LGi}\nabla c_i] = -\mathbf{u}\nabla c_i + R_{Li} + R_{Pi} + R_{Gi} + S_{ci}\end{aligned}$$

Subdomain Settings

The **Subdomain Settings** dialog box contains interfaces for: (1) **Flow and Media**, (2) **Liquid**, (3) **Solid**, (4) **Gas**, (5) **Init**, and (6) **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** tab 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 direction	
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	
dHp/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** tab 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
	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** tab 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** tab 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
A_r	Ar	Diffusion anisotropy tensor	
R_G	RG	Reaction rate, gas	

Boundary Conditions

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	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c+\mathbf{u}c) = N$ $N = \mathbf{n}\cdot\mathbf{u}c_0-\frac{D_{mG}}{d}(k_G c-c_{Gatm})$	Flow boundary volatilization
NnGatmz	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c+\mathbf{u}c) = N$ $N = -\frac{D_{mG}}{d}(k_G c-c_{Gatm})$	No flow boundary volatilization
ax	$-\mathbf{n}\cdot(-\theta D_{LG}\nabla c+\mathbf{u}c) = 0$	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 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

SYMBOL	VARIABLE	ANALYSIS	DESCRIPTION
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 3-4: APPLICATION MODE VARIABLES, SOLUTE TRANSPORT.

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	$(\alpha_1-\alpha_3)\frac{vw}{\lvert\mathbf{u}\rvert}$
thDLzz_c	All	S/B/E/P	Dispersive tensor, *zz* component	$\alpha_1\frac{w^2}{\lvert\mathbf{u}\rvert}+\alpha_3\frac{u^2}{\lvert\mathbf{u}\rvert}+\alpha_3\frac{v^2}{\lvert\mathbf{u}\rvert}+\theta\tau_L D_m$
thDLGij_c	G	S/B/E/P	Liquid Gas Dispersive tensor	$\theta D_{Lij}+a_v D_{Gij}$
avDGij_c	G	S/B/E/P	Gas Diffusion tensor	$a_v\tau_G D_{mG}A_{rij}k_G$

TABLE 3-4: APPLICATION MODE VARIABLES, SOLUTE TRANSPORT.

NAME	Mat type	**TYPE**	**DESCRIPTION**	**EXPRESSION**
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_x_i	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 3-4: APPLICATION MODE VARIABLES, SOLUTE TRANSPORT.

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	$\left\vert\frac{\mathbf{u}h}{\theta D_L}\right\vert$ (no gas) $\left\vert\frac{\mathbf{u}h}{\theta D_{LG}}\right\vert$ (gas)
dflux_c_x_i	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	$\vert\theta D_L\nabla c\vert$ (no gas) $\vert\theta D_{LG}\nabla c\vert$ (gas)
dLflux_c_x_i	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	$\vert\theta D_L\nabla c\vert$
dGflux_c_x_i	G	V	Dispersive flux, gas, x_i component	$-a_vD_G\frac{\partial c}{\partial x_i}$
dGflux_c	G	S/B/E/P	Dispersive flux, gas, norm	$\vert a_vD_G\nabla c\vert$
adflux_c_x_i	All	V	Advective flux, x_i component	cu, cv, cw
adflux_c	All	S/B/E/P	Advective flux, norm	$\vert c\mathbf{u}\vert$

TABLE 3-4: APPLICATION MODE VARIABLES, SOLUTE TRANSPORT.

NAME	Mat type	TYPE	DESCRIPTION	EXPRESSION
tflux_c_x_i	All	V	Total flux, x_i component	$-\theta D_L\frac{\partial c}{\partial x_i}+cu_i$
tflux_c	All	S/B/E/P	Total flux, norm	$\vert-\theta D_L\nabla c+c\mathbf{u}\vert$
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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