COMSOL MULTIPHYSICS

EARTH SCIENCE MODULE

MODEL LIBRARY

VERSION 3.4

COMSOL

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Earth Science Module Model Library

Version: October 2007 COMSOL 3.4

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1

Introduction

The *Earth Science Module Model Library* contains write-ups and documentation for a number of geophysical and environmental scenarios. Many of the tools discussed here will help your modeling in this module and elsewhere in COMSOL Multiphysics. We encourage you to browse and explore. An important strength of COMSOL Multiphysics is the inheritance that comes from a community of researchers across many different disciplines. Tapping into the variety available in COMSOL Multiphysics will enhance your modeling. Guaranteed.

In this library, the example models fall into five groups: fluid flow, solute transport, flow and deformation, heat transfer, and multiphysics. The models typically involve one or more application modes from the Earth Science Module. Others, such as the poroelasticity and electrokinetic volcano flow examples, utilize application modes from elsewhere in COMSOL Multiphysics. The models serve as a reference and also provide a head start for your own analyses. The ready-to-run models come with theoretical background as well as instructions that illustrate how to set it up. You can freely modify the model files, change the geometries and material properties, alter the equations, and add new physics to the file. Building on the shoulders of others saves time and adds insight.

Some models come from experts using COMSOL Multiphysics in their work and research. Others were put together by our staff engineers who have years of experience in Earth Science; they are your peers, using the language and terminology needed to get across the sophisticated concepts in these advanced topics. Many of the models have analytic solutions. Some are benchmark models designed to test the metal of dedicated physics programs.

The model descriptions range in detail. Those that describe each step are useful as tutorials. Others are in-depth examples that focus on advanced or unusual options that you can use once you are familiar with COMSOL Multiphysics modeling. Before tackling the in-depth models, we urge you to take a look at a few of the basic variety.

The *Earth Science Module User's Guide* covers the equation set up, offers some insights on the underlying physics, and includes some fundamental modeling techniques for each application mode. The *COMSOL Multiphysics User's Guide* and the *COMSOL Multiphysics Quick Start* manual provide additional information about modeling in the graphical user interface. For details about modeling with a programming language, look to the *COMSOL Multiphysics Scripting Guide*.

Each example comes with a COMSOL Multiphysics Model MPH-file that you can browse, modify and postprocess. This allows you to follow along with every step along the way whether you make the model or not. One or two of the models also includes application modes from other optional packages from COMSOL.

Model Library Guide

The table below summarizes key information about each entry in the *Earth Science Module Model Library.* The models are grouped according to the application area. The table also shows the equations used in each model. The entries with a superscript α denote models demonstrating some tools that are exceedingly useful in advanced modeling but probably offer too much challenge for a first COMSOL Multiphysics model. The Freezing Soil example utilizes an application mode from the Structural Mechanics Module denoted SME in the table.

The solution time is the elapsed time measured on a machine running Windows Vista with a 2.6 GHz AMD Athlon X2 Dual Core 500 CPU and 2 GB of RAM. For models with a sequential solution strategy, the Solution Time column shows the elapsed time for the longest solution step.

TABLE 1-1: EARTH SCIENCE MODULE MODEL LIBRARY

MODEL	PAGE	SOLUTION TIME	NAIVER-STOKES EQUATIONS	BRINKMAN EQUATIONS	DARCY'S LAW	RICHARDS' EQUATION	CONDUCTION	CONVECTION & CONDUCTION	SOLUTE TRANSPORT	OTHER
FLUID FLOW										
Pore Scale	8	24 s	√							
Finite Well	20	1 s			√					
Leaky Well	30	1 s			√					
Wellbore Storage	35	1 s			√					
Perforated Well	41	14 s			√					
Darcy-Brinkman	53	1 s		√	√					
Darcy-Brinkman–Navier-Stokes	69	27 s	√	√	√					
Discrete Fracture	85	52 s			√					
Variably Saturated Flow	99	6 s				√				
Interpolation for Unsaturated Flow	115	3 min				√				
Two-Phase Flow: Air/Water	129	6 min			√					
Two-Phase Flow: Air/Oil	129	4 min			√					
Two-Phase Flow: Oil/Water	129	5 min			√					
SOLID DEFORMATION										
Terzaghi Compaction	152	2 s			√					
Biot Poroelasticity	165	8 s			√					√
Multilateral Well	183	56 s			√					√
Freezing Soil*	198	5 min			√			√		√
SOLUTE TRANSPORT										
Solute Injection	212	3 s			√				√	
Buoyancy Flow Elder	228	47 s			√				√	
Sorbing Solute	245	23 min				√			√	
Pesticide Transport***	265	39 min				√			√	

TABLE 1-1: EARTH SCIENCE MODULE MODEL LIBRARY

MODEL	PAGE	SOLUTION TIME	NAIVER-STOKES EQUATIONS	BRINKMAN EQUATIONS	DARCY'S LAW	RICHARDS' EQUATION	CONDUCTION	CONVECTION & CONDUCTION	SOLUTE TRANSPORT	OTHER
HEAT TRANSFER										
Buoyance Free	284	2 min	√					√		
Phase Change	303	9 s					√			
Free Convection	294	24 s		√				√		
MULTIPHYSICS										
Electrokinetic Volcano 2D**	314	10 s			√					√
Electrokinetic Volcano 3D**	314	2 min			√					√

*This model requires the Structural Mechanics Module.

**This model requires the AC/DC Module.

*** This model requires the COMSOL Reaction Engineering Lab.

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.

2

Fluid Flow Models

This chapter contains a suite of models demonstrating the fluid-flow modeling capabilities in the Earth Science Module for modeling, for example, fluid flow to wells, porous media flow, and two-phase flow.

Pore-Scale Flow

This non-conventional model of porous media flow uses the Navier-Stokes equations in the interstices of a porous media. The model comes from pore-scale flow experiments conducted by Arturo Keller, Maria Auset, and Sanya Sirivithayapakorn of the University of California, Santa Barbara. To produce the model geometry they scanned electron microscope images. This type of non-conventional pore-scale modeling with COMSOL Multiphysics is shedding new light on the movement of large particulates, colloids, moving through variable-pore geometries in the subsurface. Several of these researchers have published results from their COMSOL Multiphysics modeling in the publication *Water Resources Research* (Ref. 1 and Ref. 2).

Keller, Auset, and Sirivithayapakorn designed their lab experiments on the basis of scanning electron microscope (SEM) images of thinly sliced rock sections (Figure 2-1). They etched the geometric patterns from the images onto a solid with an elaborate process similar to the etching of silicon wafers. They then transferred these images to DXF files, which they finally imported into COMSOL Multiphysics.

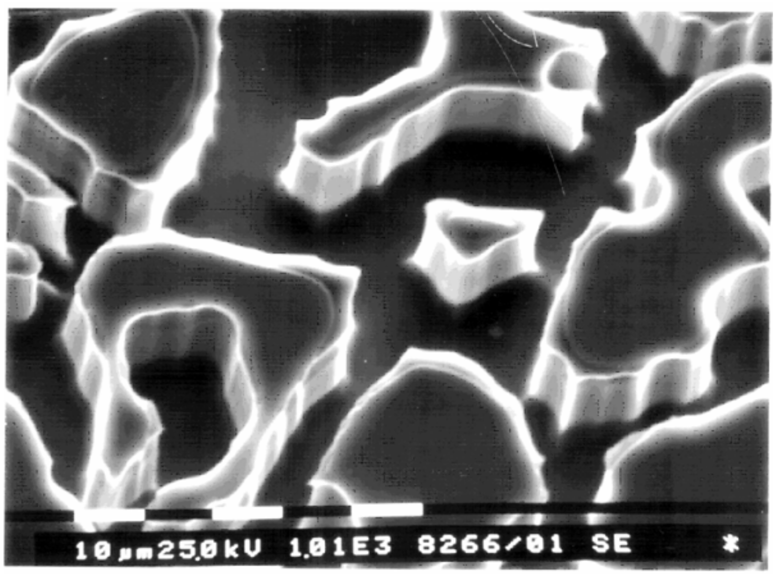


Figure 2-1: Scanning electron microscope image of the repeat pattern in the silicon wafer. The scale at bottom indicates that pore throat and body dimensions are on the order of 1 µm–100 µm (Ref. 1).

It is typical to represent fluid flow in the subsurface as a continuum process using average or "continuous" properties for the bulk rather than detailing the shape and orientation of each solid particle within a porous medium. Inserting the bulk properties into an equation such as Darcy's law gives an average flow rate for the total volume. While bulk approximations typically produce excellent estimates sufficient for considering flow over large areas, they miss the between-grain nuances that a close-up Navier-Stokes analysis describes.

This example takes one of the 2D micromedia images of Keller, Auset, and Sirivithayapakorn and solves for velocities and pressures of pore fluids using the Navier-Stokes equations for Cartesian coordinates. The exercise imports the geometry as a DXF file and does not mesh any unneeded regions. Plotting includes 3-dimensionalizing a 2D surface plot by adding height data. Boundary integration quantitatively evaluates fluxes.

Model Definition

The entire model covers 640 μm × 320 μm. Water generally moves from right to left across the geometry. Flow is laminar in the pores and does not enter the grains. The inlet and outlet fluid pressures are known. Assume flow is symmetric about the top and bottom boundaries. The primary zone of interest is the rectangular region with an upper left corner at (0, 0) μm and lower right coordinates at (581.6, –265.0) μm.

Assuming fluids in the pore spaces are at constant density and also that temperature is constant, the Navier-Stokes and continuity equations are

$$\rho\mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)]$$
$$\nabla\cdot\mathbf{u} = 0$$

where η denotes the dynamic viscosity (μg/(μm·s)), $\mathbf{u}$ represents the velocity (μm/s), ρ equals the fluid density (μg/μm^3), p denotes the pressure (μg/(μm·s)), and $\mathbf{I}$ is the identity matrix. Owing to the problem's small scale, the model does not include a body force that accounts for gravity.

The following equations give the mathematics that represent the model's physical boundaries. The inlet pressure and the outlet pressure are known. Velocities are zero at the grain boundaries, which have a no-slip condition. Flow is symmetric about the top and bottom boundaries.

$$
\begin{array}{ll}
p = p_0, \quad \mathbf{n} \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) = 0 & \text{at } \partial\Omega_{\text{inlet}} \\
p = 0, \quad \mathbf{n} \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) = 0 & \text{at } \partial\Omega_{\text{outlet}} \\
\mathbf{u} = 0 & \text{at } \partial\Omega_{\text{grains}} \\
\mathbf{n} \cdot \mathbf{u} = 0, \quad \mathbf{t} \cdot \eta(-p\mathbf{I} + \nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} = 0 & \text{at } \partial\Omega_{\text{sides}}
\end{array}
$$

In these equations, $\mathbf{n}$ is the unit normal vector, $\mathbf{t}$ is a unit tangential vector, and p_0 is a specified pressure.

Results

Figure 2-2 shows the COMSOL Multiphysics solution predicted with a Navier-Stokes analysis for the relative velocities in the pore spaces of a micro-scale porous medium. Velocities are higher in the narrowest pores than at the inlet. The fluid velocities tend to decrease in stretches where the cross-sectional area for the flow increases.

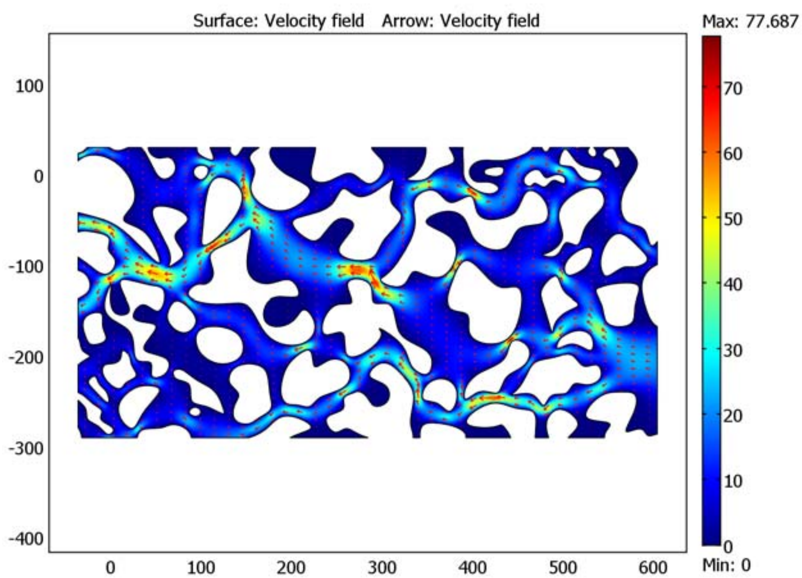


Figure 2-2: Velocity field plot showing the velocities relative to the inlet velocity within the study section.

Figure 2-3 gives the relative velocities plotted with a height that corresponds to pressure head. The figure clearly shows stagnant zones that exist within the dead-end reaches of big pores.

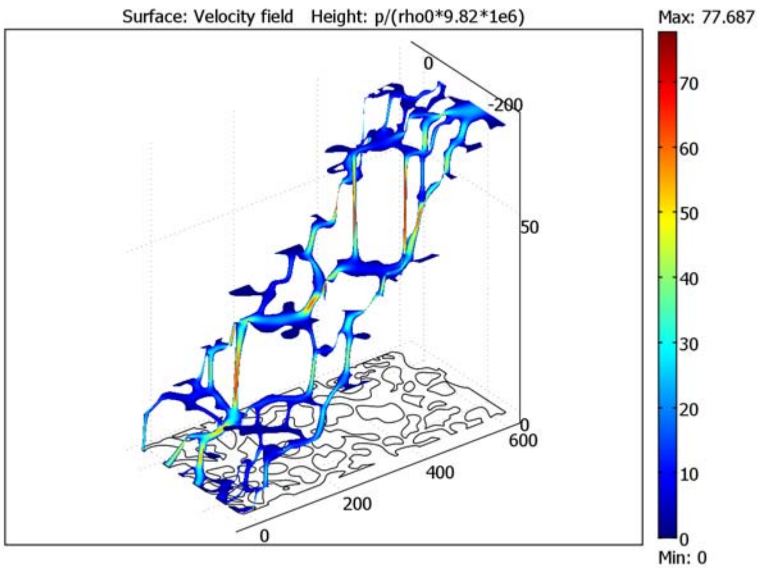


Figure 2-3: Relative velocities (represented with color, dimensionless) and pressure head (height, μm) within the study section.

The figure reveals that the highest velocities tend to occur in narrow pores with high pressure drops, as you might expect. Figure 2-4 shows a close-up view of a region near the exit, revealing that high velocities also develop in wide channels where pressure gradients are relatively shallow but multiple "tributaries" combine.

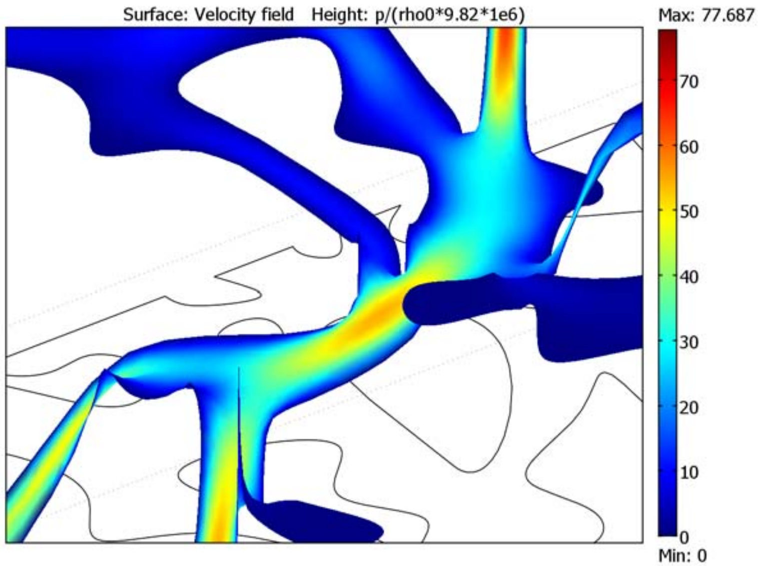


Figure 2-4: Close-up of relative velocities (color) and pressure head (height) near the outlet.

The domain plot in Figure 2-5 shows the *x*-velocity at the outlet. The velocities are negative because the flow is moving in the negative *x* direction.

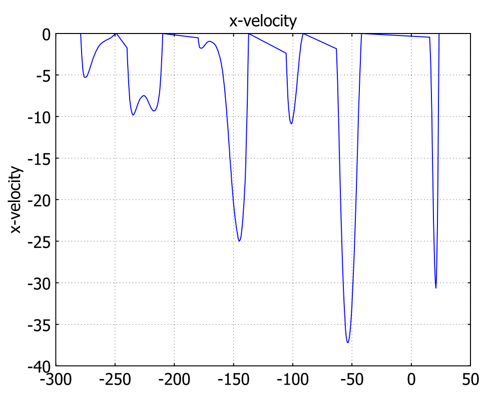


Figure 2-5: Velocities along the outlet boundaries.

References

1. M. Auset and A.A. Keller, "Pore-scale processes that control dispersion of colloids in saturated porous media," *Water Resources Research*, vol. 40, no. 3, 2004.

2. S. Sirivithayapakorn and A.A. Keller, "Transport of colloids in saturated porous media: A pore-scale observation of the size exclusion effect and colloid acceleration," *Water Resources Research*, vol. 39, no. 4, 2003.

3. A.A. Keller, M.J. Blunt, and P.V. Roberts, "Micromodel observation of the role of oil layers on multiphase flow," *Transport in Porous Media*, vol. 26, pp. 277–297, 1997.

Model Library path: `Earth_Science_Module/Fluid_Flow/pore_scale`

Modeling Using the Graphical User Interface

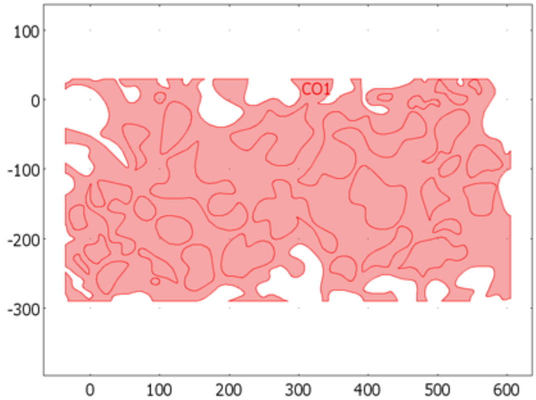
MODEL NAVIGATOR

1 Open the **Model Navigator**, and in the **Space dimension** list select **2D**.
2 From the list of application modes choose **Earth Science Module>Fluid Flow>Incompressible Navier-Stokes**. Click **OK**.

GEOMETRY MODELING

1 Import the geometry from the **DXF** file. From the **File** menu select **Import>DXF File**, then navigate to **pore_scale.dxf**.
2 Accept the default settings for the geometry import. Click **OK**.

3 From the Draw toolbar on the far left of the user interface click the **Coerce to Solid** button.



4 From the Draw toolbar select **Split Object**.

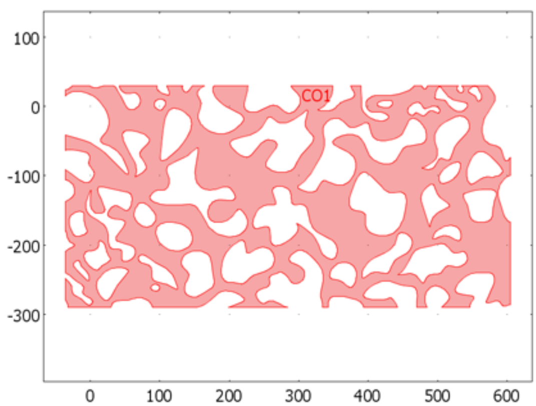
5 With the mouse, select the object CO2, the geometry object that corresponds to the open flow region.

6 Copy the geometry object by pressing Ctrl+C.

7 Select all objects by pressing Ctrl+A. Delete all objects by pressing the Delete key.

8 Paste the copied object by pressing Ctrl+V, then click **OK** in the **Displacement** dialog box that appears.

9 Click the **Zoom Extents** button on the Main toolbar to center the geometry in the field of view.



OPTIONS AND SETTINGS

1 From the **Physics** menu select **Model Settings**.
2 Clear the **Simplify expressions** check box.
3 From the **Base unit system** list select **None**, then click **OK**.
4 From the **Options** menu select **Constants**, then enter the following names and expressions; when done, click **OK**.

NAME	EXPRESSION
`rho0`	`1000*1e9/(1e6)^3`
`eta0`	`0.001*1e9/1e6`
`p0`	`715`

PHYSICS SETTINGS

Subdomain Settings

From the **Physics** menu select **Subdomain Settings**. Select Subdomain 1, then enter material properties from the following table:

VARIABLE	SUBDOMAIN 1
ρ	`rho0`
η	`eta0`

Boundary Conditions

From the **Physics** menu select **Boundary Settings**. For the various boundaries in the following table, enter the corresponding settings:

SETTINGS	BOUNDARIES 1–6	BOUNDARIES 7–25	BOUNDARIES 26, 27	ALL OTHERS
Boundary type	Outlet	Symmetry boundary	Inlet	Wall
Boundary condition	Pressure, no viscous stress	-	Pressure, no viscous stress	No slip
p_0	0		p0	

MESH GENERATION

1 From the **Mesh** menu open the **Free Mesh Parameters** dialog box, click the **Global** tab, then enter the following data:

GLOBAL MESH PARAMETERS	EXPRESSION
Maximum element size	10

GLOBAL MESH PARAMETERS	EXPRESSION
Element growth rate	`1.6`
Mesh curvature factor	`0.3`

2 On the **Boundary** page, select Boundaries 1–6. In the **Maximum element size** edit field type `3`.

3 Click the **Advanced** tab and set the **Resolution of geometry** to `20`.

4 Click the **Remesh** button, then click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 2-2 follow these steps:

1 Click the **Zoom Extents** button on the Main toolbar.

2 From the **Postprocessing** menu open the **Plot Parameters** dialog box. Click the **General** tab, then select the **Surface** and **Arrow** check boxes. Click the **Title** button, enter text as desired, then click **OK**.

3 Click the **Surface** tab. In the **Predefined quantities** list select **Velocity field**.

4 Click the **Arrow** tab. In the **Predefined quantities** list select **Velocity field**.

5 In the **Arrow positioning** area, in both the **x points** and **y points** edit fields enter `40`.

6 Click **OK**.

To generate Figure 2-3 continue with these steps:

1 Return to the **Plot Parameters** dialog box and the **General** page. Clear the **Arrow** check box (and leave the **Surface** check box remain selected).

2 Click the **Surface** tab. In the **Predefined quantities** list select **Velocity field**.

3 On the **Surface** page, click the **Height Data** tab. Select the **Height data** check box, and in the **Expression** edit field enter `p/(rho0*9.82*1e6)` to give pressure head in µm.

4 Click **OK**.

To generate Figure 2-4 continue with this step:

Define the area of interest. Go to the 3D Draw toolbar and activate the **Dolly In/Out** icon, or go to the Main toolbar and select the **Zoom Window** tool.

To generate Figure 2-5 continue with these steps:

1 From the **Postprocessing** menu open the **Domain Plot Parameters** dialog box (because you are evaluating quantities on boundaries).

2 Click the **Line/Extrusion** tab. In the **Boundary selection** list select Boundaries 1–6.

3 In the **Predefined quantities** list select **x-velocity**.

4 Go to the **x-axis** data area, and in the drop-down list select **y**. Click **OK**.

To generate particle tracing based on Stokes law continue with the following steps.

1 Open the **Constants** dialog box from the **Options** menu.

2 Add the following constants:

NAME	EXPRESSION
`pmass`	`1`
`pvol`	`4/3*pi*prad^3`
`prad`	`1`
`g`	`0`

3 From the **Solve** menu, select **Update Model**.

4 Open the **Plot Parameters** dialog box.

5 Click the **Particle Tracing** tab.

6 Type `-6*pi*prad*eta0*(partu-u)` in the **Fx** edit field.

7 Type `(pmass-rho0*pvol)*g-6*pi*prad*eta0*(partv-v)` in the **Fy** edit field.

8 Set the **Start Points** according to the following table:

START POINTS	
`x`	`linspace(600,600.001,25)`
`y`	`linspace(-80,-275.25)`

9 Click the **Initial Values** tab.

10 Set the **Initial velocity** to `u` and `v`.

11 Click the **Line Color** tab.

12 Click the **Color** button and select yellow. Click **OK**.

13 Click **OK** in the **Plot Parameters** dialog box.

Fluid Flow to Wells

Analyzing fluid flow to and from wells is critical in managing groundwater and oil resources, excavating subsurface structures, and cleaning up pollution.

The following figure shows a well withdrawing fluids from a reservoir. The well sits within a casing of relatively large diameter. The fluids moving to it are under pressure because the reservoir section that the well taps is bounded above and below, in a layer cake, by relatively impermeable materials or confining layers. The pumping generates a cone of depression in the hydraulic potential field that both expands outward and deepens with time. However, because the fluids completely fill the pore spaces, the cone of depression represents *drawdown* in the pressure potential rather than the fluid content.

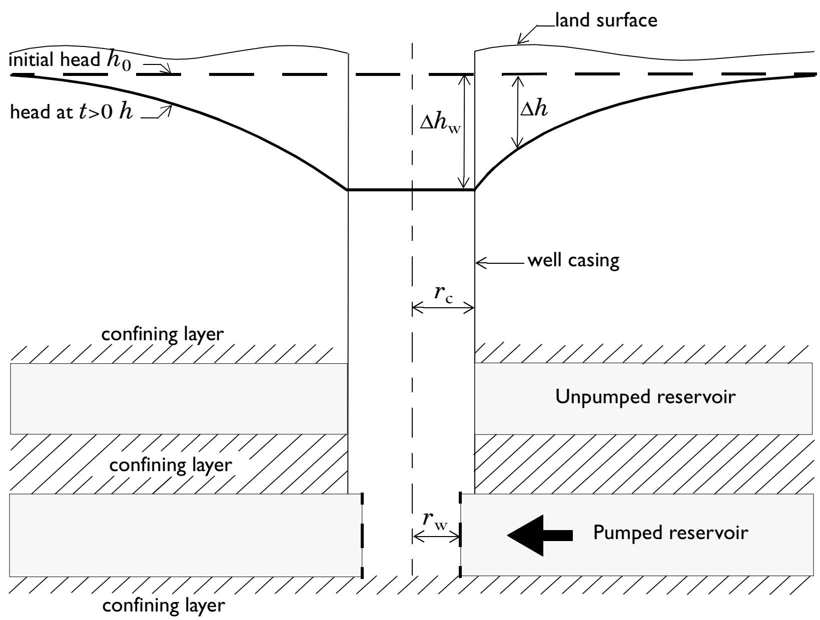


Figure 2-6: Schematic flow to a well in a confined aquifer. After Hsieh (Ref. 1).

This model demonstrates three analyses of flow to wells following lectures and class notes from Paul Hsieh of the U.S. Geological Survey and Stanford University (Ref. 1). In the first example, the well has a finite radius such that the hydraulic potential inside it equals the potential at the edge. In the second example, the confining layers make imperfect seals, so fluids from overlying reservoirs leak into the pumped aquifer. In the third analysis, the fluids inside the well or wellbore storage must be removed before reservoir fluids are extracted. This example compares COMSOL Multiphysics solutions to classic examples from Theis (Ref. 2), Hantush and Jacob (Ref. 3), and Papadopoulos and Cooper (Ref. 4).

This simple sequence of 1D axisymmetric models uses the Darcy's Law application mode from the Earth Science Module to analyze time-dependent flow to wells. The model domain is semi-infinite, but the analyses zoom in on a relatively small zone of interest and uses convenient commands for setting timed outputs over long durations.

To account for the finite well radius in the first analysis, this study extends results at the well edge over the well interior using extrusion coupling variables. To account for leakage in the second example, it adds a source term to the governing equation. To include wellbore storage impacts in the third example, you add an ordinary differential equation as boundary condition using weak formulations (with a "dweak" term). The model also demonstrates how to include externally generated solutions or data in COMSOL Multiphysics plots. For a 2D example involving a point well, see "Solute Injection" on page 212. A 3D well analysis appears in the section "Perforated Well" on page 41.

Fluid Flow to Wells: Finite Radius Well

This first example in the model sequence "Fluid Flow to Wells" on page 18 defines transient flow to a well of finite radius in a confined aquifer. This discussion then compares the results from this analysis to the well-known solution for flow to a point well (Theis, Ref. 2). What distinguishes this model from the Theis problem is the well geometry because the analytical solution describes the well as a point source that produces unphysical results inside the wellbore. The COMSOL Multiphysics analysis produces a physically based solution in the well using extrusion-coupling variables to extend the results at the well edge over the well interior.

Apart from the well geometry, assumptions underlying the Theis problem apply. The reservoir is of infinite horizontal extent and is confined above and below by impermeable layers. As the well fully penetrates the reservoir, withdrawals are uniform along its length, making flow entirely horizontal. The problem neglects storage in the well. Fluids are released instantaneously from storage in the aquifer. Prior to pumping, the flow field is at steady state. Flow is horizontal, does not vary with depth, and equipotentials are axisymmetric about the wellhead.

Taking advantage of symmetry, you can approximate the semi-infinite aquifer as a long line, here 10 km. A 1-km segment represents the zone of interest. The well radius is 0.1 m. The hydraulic conductivity, K, is 10^{-4} m/s, and the thickness, b, is 50 m. The storage coefficient for pressure, S (m·s^2/kg), equals $\mathrm{Ss}/\rho_{\mathrm{f}} g$. Ss is the specific storage for hydraulic head of 10^{-5} m^{-1}, ρ_f represents the fluid density (kg/m^3), and g is gravity (m/s^2). The pumping rate, W, of 0.05 m^3/s is constant. The initial pressure, p_0, is $9.82 \cdot 10^5$ Pa. The period of interest is 10^7 s or roughly four months.

Model Definition

You typically define fluid flow in the subsurface by inserting Darcy's law for fluid velocity into an equation of continuity. For a dependent variable of pressure p (kg/(m·s^2)), the governing equation reads

$$S\frac{\partial p}{\partial t} + \nabla \cdot \left[-\frac{K}{\rho_{\mathrm{f}} g}\nabla(p + \rho_{\mathrm{f}} g D)\right] = Q_s\,.$$

The equation builds on the storage coefficient S ($m \cdot s^2/kg$), K is the hydraulic conductivity (m/s), D denotes the vertical coordinate (m); and Q_s is a volumetric flow rate per unit volume of aquifer (1/s). In this analysis you set D to zero because the analysis is 1D horizontal.

The drawdown, d_r (m), is

$$d_r = \frac{p_0 - p}{\rho_f g}$$

where p_0 is the pressure at the onset of pumping. Fluid moves into the well with a velocity described by Darcy's law

$$-\frac{K}{\rho_f g}(\nabla p + \rho_f g D) = \frac{W}{2\pi r_w b}$$

where W is the volumetric pumping rate, W ($1/(m^3 \cdot s)$) for a cylindrical wellbore, r_w represents the well radius, and b gives the vertical length of the pumping interval, in this case the aquifer thickness. The distill boundary is sufficiently far from the well that the pumping does not affect it.

The boundary and initial conditions for this model are:

$$\begin{array}{ll} \mathbf{n} \cdot \left[-\frac{K}{\rho_f g}\nabla p\right] = -\frac{W}{2\pi r_w b} & \partial\Omega \;\; \text{Well} \\ p = p_0 & \partial\Omega \;\; \infty \\ p = p_0 & t = 0 \end{array}$$

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

Implementation: Extrusion Coupling Variables

The finite element method is sufficiently robust to estimate the pressure precisely at the well screen, $r = r_w$, rather than averaging over a square (finite difference) or reducing the well to a point (analytic). Because pressure is continuous in fluids, the pressure inside the well equals the pressure just outside of it.

This axisymmetric model begins at the center of the well, at $r = 0$. If you "turn off" equations inside the well, where $r < r_w$, the well screen becomes a boundary. To see the pressure in the well, extrude the solution at r_w through the well interior using coupling variables. Extrusion-coupling variables take information from one type of model domain (such as the boundary at the well radius) and extrude it over other domain types (such as the subdomain inside the well). This can be very powerful modeling feature. For example, with coupling variables you can express material properties that depend on the solution at some critical zone in the model, or define one boundary using results for another to give identical conditions. For more information on coupling variables, refer to "Using Coupling Variables" on page 255 of the *COMSOL Multiphysics User's Guide*.

Results

Figure 2-7 illustrates the COMSOL Multiphysics solution for flow to a finite radius well. The results at varying times for a 1000-m extent show the cone of depression the pumping produces. Because the solution never reaches steady state, pressures drop with time.

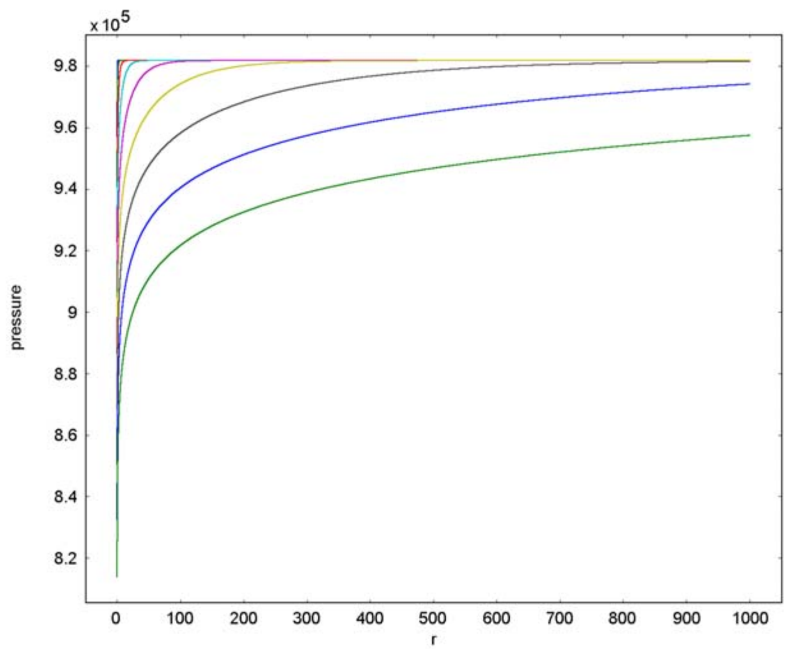


Figure 2-7: COMSOL Multiphysics solution for fluid pressure near a finite radius well along the line r < 1000 m. Results are for logarithmically spaced times from 0 ≤ t ≤ 11.5 days.

Figure 2-8 plots the solution as drawdown versus time at five points in the aquifer; it also gives the Theis estimates for drawdown. Unlike the pressure solution, the drawdown increases with time and decreases with distance from the well. The author calculated the Theis estimates within COMSOL Multiphysics and added them to the plot.

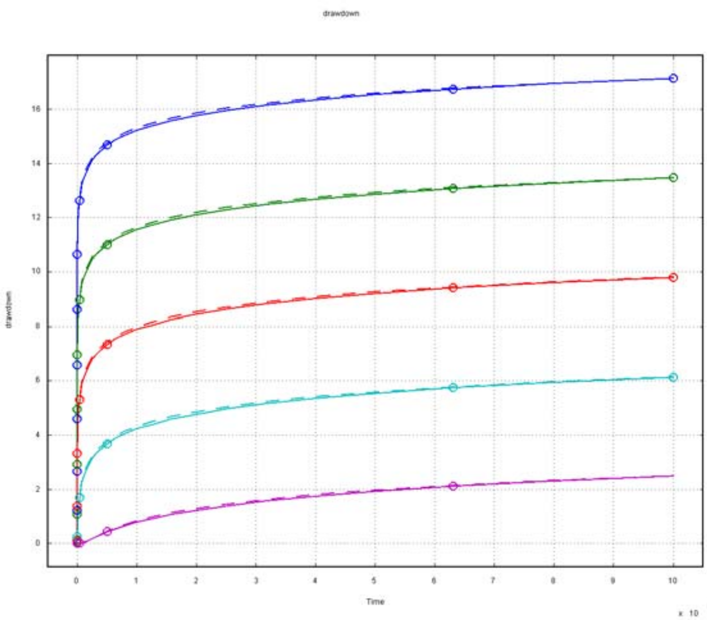


Figure 2-8: COMSOL Multiphysics results (solid lines with circles) shown with the Theis (Ref. 2) analytic solution (dashed lines) for drawdown in the aquifer at $r = r_w$, 1 m, 10 m, 100 m, and 1000 m.

The COMSOL Multiphysics and Theis estimates are very similar outside the well. What happens inside the well, however, is critical in many analyses. Figure 2-9 is a close-up view showing that COMSOL Multiphysics gives a physically-based solution inside the wellbore. The analytic estimates change unrealistically inside the wellbore because they represent withdrawals from a point.

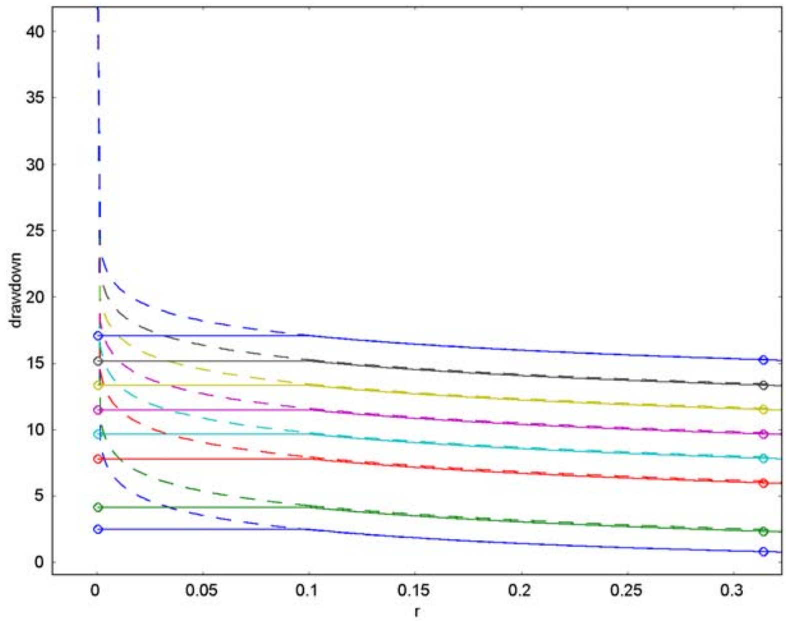


Figure 2-9: COMSOL Multiphysics drawdown solution for the finite radius well (solid lines with circles) shown with the Theis estimates for a point well (dashed lines) along the line $r < 0.3$ m.

The solution at the well radius appears inside the wellbore via extrusion-coupling variables from COMSOL Multiphysics.

References

1. P. Hsieh, course notes for GES 236—Hydraulic and Tracer Tests for Groundwater Resource Evaluation, Stanford University, 2003, http://pangea.stanford.edu/hydro/classes/GES236/236notes.htm

2. C.V. Theis, "The relationship between the lowering of the piezometric surface and the rate and duration of discharge of a well using ground-water storage," *Transactions American Geophysical Union*, vol. 16, 1935.

3. M.S. Hantush and C.E. Jacob, "Nonsteady radial flow in an infinite leaky aquifer," *EOS Transactions American Geophysical Union*, vol. 36, no. 1, pp. 95–100, 1955.

4. I.S. Papadopoulos and H.H. Cooper Jr., "Drawdown in a Well of Large Diameter," *Water Resources Research*, vol. 3, no. 1, 1967.

Model Library path: `Earth_Science_Module/Fluid_Flow/finite_well`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**. From the **Space dimension** list select **Axial symmetry (1D)**.

2 In the list of application modes select **Earth Science Module>Fluid Flow>Darcy's Law>Pressure analysis>Transient analysis**. Click **OK**.

GEOMETRY MODELING

1 From the **Draw** menu select **Specify Objects>Line**.

2 In the **Coordinates: x** edit field enter `0 0.1 1000 10000`. Click **OK**.

3 On the Main toolbar click the **Zoom Extents** button.

OPTIONS AND SETTINGS

1 Select the menu item **Options>Constants**, then enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rhof	1000[kg/m^3]	Fluid density
Ks	1e-4[m/s]	Hydraulic conductivity
Ss	1e-5[1/m]	Specific storage for hydraulic head
W	0.05[m^3/s]	Pumping rate
b	50[m]	Thickness
rw	0.1[m]	Well radius
p0	9.82e5[Pa]	Initial pressure

2 Select the menu item **Options>Expressions>Scalar Expressions**, then define the following names and expressions; when done, click **OK**.

NAME	EXPRESSION
`Theis`	`W/(4*pi*Ks*b)*Wu`
`u`	`Ss*r^2/(4*Ks*t)`
`Wu`	`(-0.5772+u-0.25*u^2+0.055*u^3-0.01*u^4+0.001*u^5-log(u))*(u<1)+(exp(-u)*(u^4+8.58*u^3+18.06*u^2+8.64*u+0.27)/(u^4+9.57*u^3+ 25.63*u^2+21.1*u+3.96)/u)*(u>=1)`

3 Open the menu item **Options>Expressions>Subdomain Expressions** and define the names on the indicated domains; when done, click **OK**.

NAME	SUBDOMAIN 1	SUBDOMAINS 2, 3
`pressure`	`pwell`	`p`
`drawdown`	`(p0-pwell)/(rhof*g_esdl)`	`(p0-p)/rhof/g_esdl`

4 Open the menu item **Options>Extrusion Coupling Variables>Boundary Variables** and enter the following settings:

SOURCE	NAME	EXPRESSION	TRANSFORMATION
Boundary 2	`pwell`	`p`	General

5 Still in the same dialog box, click the **Destination** tab and choose the following:

LEVEL	SUBDOMAIN SELECTION
Subdomain	1

6 Click **OK**.

PHYSICS SETTINGS

Application Scalar Variables

Select the menu item **Physics>Scalar Variables** and change the elevation coordinate to zero (because the model is 1D axisymmetric in the horizontal), then click **OK**.

NAME	EXPRESSION
D_esdl	0

Subdomain Settings

1 From the **Physics** menu open the **Subdomain Settings** dialog box, then select Subdomain 1. Clear the **Active in this domain** check box. When the subdomain is deactivated, the check box should be empty.

2 Select Subdomains 2 and 3, then from the **Storage term** list select **User defined**. Go to the other drop-down list and change the setting from **Permeability** to **Hydraulic conductivity**. Enter the following expressions:

PROPERTY	EXPRESSION
S	`Ss/(rhof_esdl*g_esdl)`
K_s	`Ks`

3 Click the **Init** tab, and in the **Initial value** edit field enter `p0`. Click **OK**.

Boundary Conditions

From the **Physics** menu select **Boundary Settings**, then enter the following boundary conditions; when done, click **OK**.

CONDITION	VARIABLE	BOUNDARY 2	BOUNDARY 4
Inward flux	N_0	`-W/(2*pi*rw*b)`	
Pressure	p_0		`p0`

MESH GENERATION

1 From the **Mesh** menu select **Free Mesh Parameters**.

2 Click the **Subdomain** tab, select Subdomain 2, then in the **Maximum element size** edit field enter `10`.

3 Click the **Boundary** tab, select Boundary 2, and in the **Maximum element size** enter `0.001`. Click **OK**.

COMPUTING THE SOLUTION

1 From the **Solve** menu open the **Solver Parameters** dialog box. Verify in the **Solver** list that **Time dependent** is selected.

2 To specify output times for the model, click on the **General** tab and go to the **Time-stepping** area. In the **Times** edit field enter `0 logspace(-2,6,81)` to generate output data at time zero and also at 81 logarithmically spaced times from 10^{-2} to 10^6 time units. Click **OK**.

3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 2-7 proceed as follows:

1 From the **Postprocessing** menu select the **Domain Plot Parameters** dialog box.

2 In the **Solution to use** list select **0.1**, **1**, **10**, **1e2**, **1e3**, **1e4**, **1e5**, and **1e6**. Click the **Title/ Axis** button and enter a title as appropriate.

3 Click the **Line/Extrusion** tab. In the list of **Predefined quantities** select **Pressure**. Then choose Subdomains 1 and 2. Click **OK**.

To generate Figure 2-8, continue with these steps:

1 From the **Postprocessing** menu select **Cross-Section Plot Parameters**. In the resulting dialog box click on the **Point** tab, then find the **y-axis data** area. In the **Expression** edit field enter `drawdown`. In the **Coordinates** area go to the **r** edit field and enter `0.1 10 100 100`. Click **Apply**.

2 Click the **General** tab, then select the **Keep current plot** check box.

3 Return to the **Point** tab, and in the **Expression** edit field enter `Theis`. Click the **Line Settings** button; in the **Line style** list select **Dashed line**, and in the **Line marker** list select **Circle**. Click **OK**, then click **Apply**.

4 Focus in on the results for r < 100 m using the rubber-band tool you access with the **Zoom Window** button on the Main toolbar.

To generate Figure 2-9, continue with these steps:

1 From the **Postprocessing** menu select **Domain Plot Parameters**, then click the **Line/ Extrusion** tab. Go to the **y-axis data** area and in the **Expression** edit field enter `drawdown`. Click the **Line Settings** button and modify the line appearance as appropriate.

2 Click the **General** tab. In the **Solutions to use** list select **0.1 1 10 100 100 10000 100000** and **1000000**. Make sure the **Keep current plot** check box is selected. Click **Apply**.

3 Return to the **Line/Extrusion** tab and in the **Expression** edit field enter `Theis`. Click the **Line Settings** button, and change the line settings as appropriate, click **OK**, then click **Apply**.

4 Zoom in on the results for r < 0.3 m using the rubber band tool you access with the **Zoom Window** button on the Main toolbar. Click **OK**.

SAVING THE MODEL

This completes the initial well model. You will add new equations and terms in the next sections. To use this model for the next two analyses, please save it by going to

File>Save As and entering an appropriate file name. Click **OK**. Then leave the model file open.

Fluid Flow to Wells: Leaky Well

In layered sedimentary sequences, confining units often sandwich viable reservoirs. Such is the case in Figure 2-6. If the confining units create less than perfect seals, fluids from an overlying reservoir can leak into the pumped reservoir below it. Often the pumping from the lower reservoir does not change flow in the unpumped one above. In these cases you can model the leakage through the imperfect confining unit as a distributed source of fluid to the lower reservoir, in the same fashion as recharge or precipitation.

This example is the second model in the series overviewed in "Fluid Flow to Wells" on page 18. This analysis builds on the example "Fluid Flow to Wells: Finite Radius Well" on page 20 to simulate pumping from a leaky aquifer. The discussion compares COMSOL Multiphysics results to the analytic problem of Hantush and Jacob (Ref. 1). The 3-part analysis builds on a lecture series from Hsieh (Ref. 2).

Model Definition

The governing equation for this problem is

$$S\frac{\partial p}{\partial t} + \nabla \cdot \left[-\frac{K}{\rho_f g}\nabla p\right] = \frac{K'}{\rho_f g}\frac{(p_0 - p)}{bb'}$$

where K' $(1/(\mathrm{m \cdot s}))$ and b' (m) are the hydraulic conductivity and thickness of the overlying confining unit, respectively. With p_0 being the pressure prior to pumping, the term $K'(p_0 - p)/(bb')$ amounts to Darcy's law for flow through the semi-pervious confining unit. The thickness of the pumped reservoir b appears in the denominator because the incoming fluid is distributed through the aquifer volume.

The boundary and initial conditions are the same as in the finite-well model:

$$\begin{aligned}
\mathbf{n} \cdot \left[\frac{K}{\rho_f g}\nabla p\right] &= \frac{W}{2\pi r_w b} && \partial\Omega \ \text{ well} \\
p &= p_0 && \partial\Omega \ \infty \\
p &= p_0 && t = 0.
\end{aligned}$$

The geometry, the material properties, and the pumping rates come from the finite-well flow model. To describe the leakage through the confining layer, you specify its hydraulic conductivity, K', as $5 \cdot 10^{-8}$ m/s and its thickness, b', as 2 m.

Results

Figure 2-10 shows the COMSOL Multiphysics solution for the distribution of pressures in a pumped aquifer with leakage from an overlying layer. Even for a relatively impermeable confining unit with hydraulic conductivity $K' = K/100$, the leakage is significant. For example, this figure depicts a far less extensive cone of depression than the one in Figure 2-7 which characterizes pumping in the same aquifer but without the leakage.

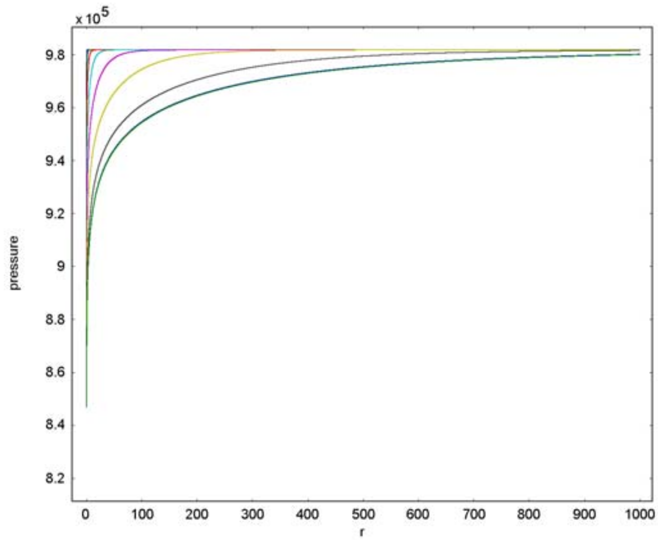


Figure 2-10: Solution for the fluid pressure near a finite-radius well in a leaky aquifer. Results are for logarithmically spaced times from $0 \leq t \leq 11.5$ days along the line $r < 1000$ m.

The plot in Figure 2-11 converts the solution to the leaky aquifer to drawdown (defined on page 21) and plots it against time; it also shows the results for the case without leakage from Figure 2-8. The later time drawdown for the leaky case is almost constant by comparison. At early times, fluid reaching the wells comes from the storage in the pumped reservoirs. At later times, fluids pumped from the leaky aquifer derive mostly from the unpumped aquifer above it.

Figure 2-11 also provides the analytic solution of Hantush and Jacob (Ref. 1). The COMSOL Multiphysics results are good fit to the analytic solution.

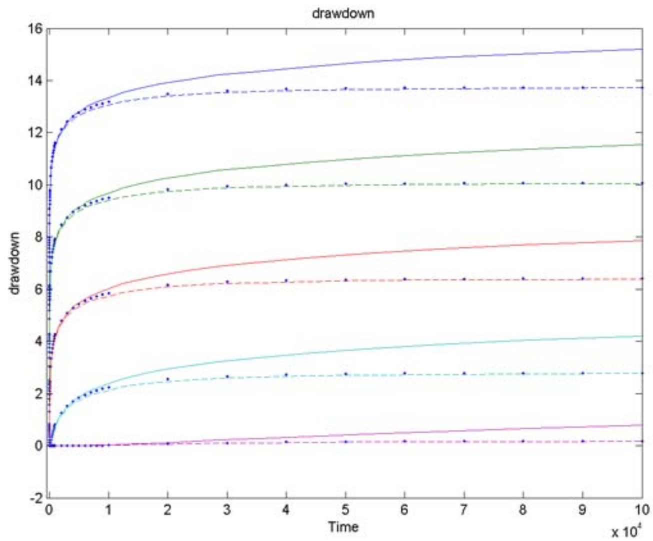


Figure 2-11: COMSOL Multiphysics drawdown estimates for a leaky confined aquifer (dashed lines) compared with the analytic solution (dots) from Hantush and Jacob (Ref. 1). Also shown are results of simulations without the leakage (solid lines). Results are for $r = r_w$, 0.1 m, 1 m, 10 m, 100 m, and 1000 m.

References

1. M.S. Hantush and C.E. Jacob, “Nonsteady radial flow in an infinite leaky aquifer,” *EOS Transactions American Geophysical Union*, vol. 36, no. 1, pp. 95–100, 1955.

2. P. Hsieh, course notes for GES 236—Hydraulic and Tracer Tests for Groundwater Resource Evaluation. Stanford University, 2003 http://pangea.stanford.edu/hydro/classes/GES236/236notes.htm.

Model Library path: `Earth_Science_Module/Fluid_Flow/leaky_well`

MODEL NAVIGATOR

1 Open the **Model Navigator**, and click the **Model Library** tab.

2 Open the **Earth Science Module** folder.

3 Find the **Fluid Flow** folder and select the file **finite well**.

4 Click **OK**.

PRELIMINARIES

Before adding to the model, create a cross-section plot of the results already in memory for use in a comparison plot with results from the modified model.

From the **Postprocessing** menu open the **Cross-Section Plot Parameters** dialog box. Click the **Point** tab, and in the **Expression** edit field enter `drawdown`. In the **Coordinates: r** edit field enter `0.1 1 10 100 1000`. Click **Apply**. Leave the plotting window open.

OPTIONS AND SETTINGS

From the **Options** menu open the **Constants** dialog box, then add these names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
Kpr	5e-8[m/s]	Hydraulic conductivity of confining layer
bpr	2[m]	Thickness of confining layer

SUBDOMAIN SETTINGS

From the **Physics** menu open the **Subdomain Settings** dialog box. Select Subdomains 2 and 3, then enter the following name and expression; when done, click **OK**.

NAME	EXPRESSION
Qs	Kpr/(rhof*g_esdl)*(p0-p)/(b*bpr)

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 2-10, follow the instructions for Figure 2-7 already given.

To create Figure 2-11, first add the current results to Figure 2-8 and later the analytic solution. To add the current results to Figure 2-8, follow these steps:

1 From the **Postprocessing** menu open the **Cross Section Plot Parameters** dialog box. On the **General** tab, click the **Titles/Axis** button and provide new titles for the plot as appropriate, then click **OK**. Make certain that the **Keep current plot** check box is selected. If you run COMSOL Multiphysics with MATLAB, choose **MATLAB Figure** for the new plot.

2 Click the **Point** tab, then in the Expression edit field enter `drawdown`. Make sure the expression in the **Coordinates** edit field is `0.1 1 10 100 1000`. Click **Apply**.

If you have COMSOL Script or MATLAB, you can add the analytic solution.

3 Go the command line and enter the following code:

```
hold on
load leaky_analytic.txt
t = leaky_analytic(:,1);
A = leaky_analytic(:,2);
plot(t,A,'.')
```

the file `leaky_analytic.txt` should be available in your path.

4 Edit the figure axis and line settings as needed.

Fluid Flow to Wells: Wellbore Storage

Pumping from a finished well removes whatever fluids are in the well and the casing around it before fluids from the reservoir enter the well. The magnitude and duration of the wellbore storage's impact is related to the size of the well and casing. These effects stand out particularly at early times, typically when engineers assess the viability of reservoirs. For large-scale projects with big wells, these "early time" effects can linger for many months and significantly inhibit production.

Wellbore storage effects have been the subject of much study in hydrogeology and petroleum engineering. Being particularly difficult to analyze, they are rarely considered in conventional numerical models. This section models wellbore storage by adding a time-dependent ordinary differential equation to the well boundary. The results shown here match the analytic solution of Papadopoulos and Cooper (Ref. 1). The method this analysis uses extends to account for skin effects.

Model Definition

This analysis of wellbore storage is the final example in the sequence described in "Fluid Flow to Wells" on page 18. It builds directly on the 1D axisymmetric model "Fluid Flow to Wells: Finite Radius Well" on page 20. As before, the equation governing the flow is

$$S\frac{\partial p}{\partial t} + \nabla \cdot \left[-\frac{K}{\rho_f g}\nabla p\right] = Q_s$$

What changes is the mathematical model for flow at the well. The expression used here accounts for wellbore storage as follows:

$$W = -\frac{K}{\rho_f g}2\pi r_w b \nabla p|_{r = r_w} + \frac{\pi r_c^2}{\rho_f g}\frac{dp_w}{dt}$$

where r_c is the radius of the well casing; and $p_w(t)$, normalized by the specific gravity $\rho_f g$, is drawdown in the well. This equation states that withdrawals from the well consist of two parts: First is the flux into the well from the aquifer, and second is the water coming from the wellbore itself. The foregoing specifies that the pressure just inside the well, $p_w(t)$, equals the pressure just outside of it, $p(r_w, t)$. In other words, $p_w(t) = p_w(r_w, t)$. A skin effect produces a discontinuity in pressure from just inside the well to just outside of it. To model the discontinuity, you also would add a third term to account for the step change.

The boundary and initial conditions for the Wellbore Storage model are

$$\mathbf{n} \cdot \left[-\frac{K}{\rho_f g}\nabla p\right] = -\left(W + \frac{\pi r_c^2}{\rho_f g}\frac{dp_w}{dt}\right)(2\pi r_w b)^{-1} \qquad \partial\Omega \ \text{Well}$$

$$p = p_0 \qquad \partial\Omega \ \infty$$

$$p = p_0 \qquad t = 0$$

where **n** is the normal to the boundary.

To simplify this analysis, use material properties and pumping rates from the original Finite Well model and add the radius of the well casing, r_c (set to 0.15 m as a start). With this parameterization, interesting results occur very early. To zoom in on these results you can reduce the simulation period.

Results

Figure 2-12 shows the COMSOL Multiphysics solution for drawdown as a function of time for five observation points near a well with wellbore storage impacts. The figure also provides results for the case without wellbore storage (see Figure 2-8). The difference in the two solutions is the reduction in reservoir withdrawals owing to fluids present in the wellbore. This impact, as expected, diminishes with distance and time.

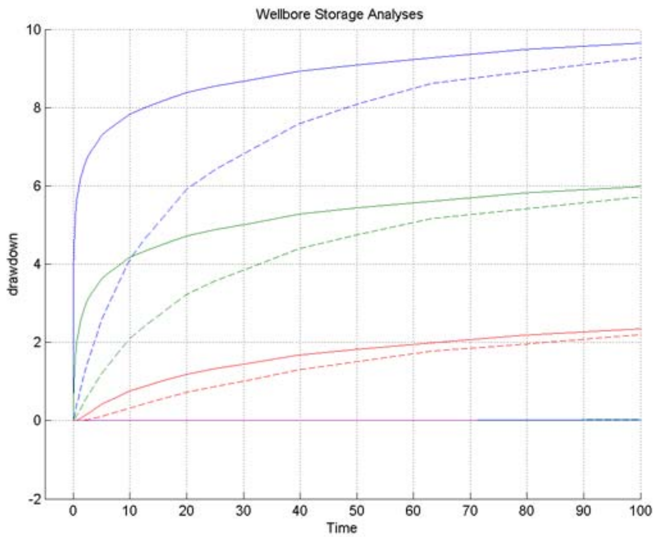


Figure 2-12: Drawdown estimates predicted with (dashed lines) and without (solid lines) wellbore storage. Results are for the well boundary and points at increasing distance from it.

Figure 2-13 compares a time series of drawdown from simulations including wellbore storage with different casing radii. COMSOL Multiphysics gives a near-perfect match to the analytic solution in Ref. 1. The solid line corresponds to the solution without wellbore storage. The next curve (dashed line) corresponds to a well casing with the same radius as the screened interval. Subsequent curves are for increasing casing radii. The plot shows that as the casing radius increases, the pumping removes less and less fluid from the reservoir for longer and longer times.

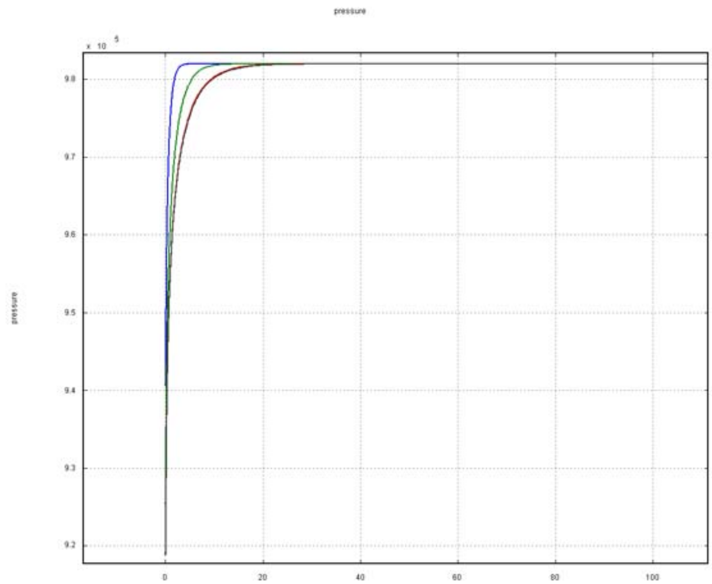


Figure 2-13: Drawdown at the well for increasing well-casing radii (dashed lines) and without wellbore storage impacts (solid lines). The results almost exactly match the analytic solution of Papadopoulos and Cooper (Ref. 1).

Reference

1. I.S. Papadopoulos and H.H. Cooper Jr., "Drawdown in a Well of Large Diameter," *Water Resources Research*, vol. 3, no. 1, 1967.

Model Library path: `Earth_Science_Module/Fluid_Flow/wellbore_storage`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator** and click the **Model Library** tab.

2 Find the file **Earth Science Module>Fluid Flow>finite well**.

3 Click **OK**.

OPTIONS AND SETTINGS

From the **Options** menu open the **Constants** dialog box, then add the following name, expression, and description (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rc	0.15[m]	Radius of the well casing

PHYSICS SETTINGS

Boundary Settings

1 From the **Physics** menu open the **Boundary Settings** dialog box and remove the previous boundary condition on the well. To do so, go to the **Boundary selection** list and choose **2**.

2 In the **N_0** edit field for **Inward flux** enter `-(W+pi*rc^2*pt/(rhof_esdl*g_esdl))/(2*pi*rw*b)`. Click **OK**.

COMPUTING THE SOLUTION

1 To solve the wellbore storage model, go to the menu item **Solve>Solver Parameters** dialog box and change the output time expression in the **Times** edit field to `0 logspace(-3,2,101)`.

2 Solve the model as before by clicking the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The steps to generate Figure 2-12 follow the instructions outlined for Figure 2-11 in the previous model.

It is advisable to regenerate the original solution for the plot. To do so, go to the **Options>Constants** dialog box, change the r_c value to zero, then solve the problem.

To generate Figure 2-13, follow these steps:

1 From the **Postprocessing** menu open the **Cross-Section Plot Parameters** dialog box. Click the **Point** tab, go to the **y-axis data** area, and check that the value in the **Expression** edit field is `drawdown`; if not, enter it. In the **Coordinates: r** edit field enter `0.1`. Click **Apply**.

2 To add results from a number of simulations for different well casing radii r_c, click the **General** tab and select the **Keep current plot** check box.

3 Now you change the value of r_c for a given run and then solve and add the results of that simulation to the plot. Then repeat. For example, select the menu item **Options>Constants** and first change r_c to 0. Click **Apply.** Then you solve as before and

plot the results for each solution. This example uses $r_c = 0, 0.1, 0.15, 0.2, 0.25$, and 0.3.

4 Click **OK**.

Perforated Well

Analysis of fluid flow into wells often begins with the assumption that the intake of fluid is uniform along the entire length of wellbore. This assumption runs into trouble when applied to the modeling of perforated wells. When engineers emplace these wells they line a deep bore hole with impermeable materials. Later a machine pierces the lining so the well takes in fluids in the productive reservoir zones and nowhere else. The perforations are relatively small, typically less than 0.5 m long and with a diameter of less than 5 cm. They are typically oriented at regular intervals cycling down the casing axis.

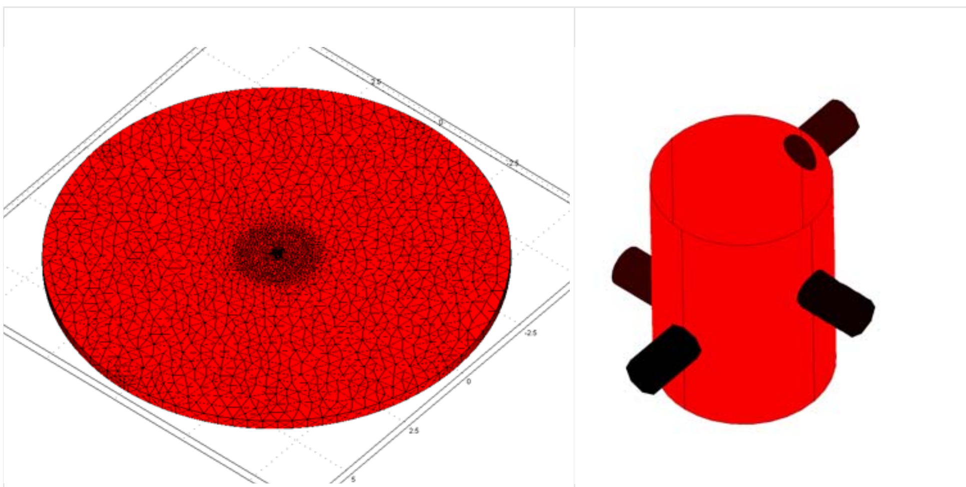


Figure 2-14: Meshed model geometry (radius 6 m, height 0.3 m) with a close-up view of the wellbore (radius 0.1 m, height 0.3 m) with cylindrical perforations. (The geometry and mesh are from Dr. M. Jamiolahmady, Institute of Petroleum Engineering, Heriot-Watt University.)

The ability to describe how fluids funnel into tiny perforations oriented about a wellbore is the subject of a rapidly growing number of analyses including those in Ref. 1, Ref. 2, and Ref. 3. Because the perforations are isolated piercings as opposed to rings, the flow field is not suited for axisymmetric analyses—fully 3D simulations are required.

This model characterizes 3D flow to a perforated well using the Darcy's Law application mode. The analysis is based on a geometry contributed by the Institute of

Petroleum Engineering at Heriot-Watt University. Dr. Jamiolahmady, an expert in non-Darcy flow, used a MATLAB script to produce and mesh incrementally different geometries for iterative simulation and analyses. The script is available for you to use and modify (get it from your COMSOL customer service representative), although you can also build the geometry using the COMSOL Multiphysics graphical user interface. Readers interested in applying an iterative simulation approach can employ parametric solutions in COMSOL Multiphysics or scripting with MATLAB.

This example demonstrates several useful COMSOL Multiphysics features. Included are instructions for using Lagrange multipliers to calculate a high-accuracy flux on a relatively low density mesh. The model also shows how to set up boundary-integration coupling variables to automate flux calculations. The following sections provide an overview of the model, and following it come tabulated on parameter values.

Model Definition

In this model, a well sits at the center of a thin (roughly 0.25 m), horizontal production reservoir that is confined above and below by impermeable units (Figure 2-14). For simplicity, the producing zone is homogeneous and isotropic with respect to permeability and porosity, and the oil has constant density and viscosity. The geometry is a reach of reservoir with a radius of approximately 6 m, which by design is 60 times greater than the well radius of 0.1 m. The model assumes that the oil moving into the well comes uniformly from the reservoir circumference, and the pressure is known at all perforations. Pumping proceeds initially at a given rate. The withdrawals come strictly through the perforations. This example contains an analysis of a steady flow field.

Darcy's law defines the velocity in the continuity equation that governs this problem. For a dependent variable of pressure, the governing equation reads

$$\nabla \cdot \left[-\frac{\kappa}{\eta}\nabla(p + \rho_f g D)\right] = Q_s$$

where κ is permeability (m^2); η represents dynamic viscosity (kg/(m·s)); ρ_f is the fluid density (kg/m^3); g equals the acceleration of gravity (m/s^2); D denotes the coordinate for vertical elevation (m); and Q_s is the volumetric flow rate per unit volume of reservoir for a fluid source (1/s).

At steady state, the flux through the circumference of the reservoir must satisfy the withdrawal at the well. Described by Darcy's law, the flux is

$$-\frac{\kappa}{\eta}(\nabla p) = \frac{W}{2\pi r_{\mathrm{res}} b}$$

where W is the volumetric pumping rate $(1/(\mathrm{m}^3 \cdot \mathrm{s}))$; r_{res} gives the reservoir radius (m); and b is the length of the well interval that takes in fluids (the so-called production interval).

Because all other boundaries are impermeable to flow, the boundary conditions are

$$\begin{array}{ll}
\mathbf{n} \cdot \left[\frac{\kappa}{\eta}(\nabla p)\right] = -\frac{W}{2\pi r_{\mathrm{res}} b} & \partial\Omega \;\; r_{\mathrm{res}} \\
p = p_{\mathrm{well}} & \partial\Omega \;\; \text{perforations} \\
\mathbf{n} \cdot \left[\frac{\kappa}{\eta}(\nabla p)\right] = 0 & \partial\Omega \;\; \text{casing} \\
\mathbf{n} \cdot \left[\frac{\kappa}{\eta}(\nabla p)\right] = 0 & \partial\Omega \;\; \text{confining layer}
\end{array}$$

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

COMSOL Multiphysics Implementation—Boundary Flux

In this model you calculate the flux through the perforations using boundary integration-coupling variables. You can perform integration as a postprocessing step from the COMSOL Multiphysics menus, but creating the variables automates the calculations and also makes the results available for plotting.

Integration coupling variables give the value of an integral over a boundary, a subdomain, or a point (the source domain); they also transmit the information from one domain to, for example, other boundaries, subdomains, and points (the destination domain). You calculate the total flux through all of the perforation boundaries with the relationship

$$\mathrm{flux} = \sum \int \left| \mathbf{n} \cdot \frac{\kappa}{\eta} \nabla p \right| \partial\Omega$$

where Ω represents the boundary. This equation takes the absolute value because the flux is everywhere an outflow, but the normals to the perforations do not all point in the same direction. To know more about the normals to boundaries, consider the following. In a simple model geometry, such as a rectangle, it is straightforward that the normals should point outward. If you add a complicated geometry inside the rectangle, where should the normals point? There is no unambiguously universal rule.

You can visualize normals to boundaries by plotting them as arrows—specify `nx`, `ny`, and `nz` in the vector expression fields for boundary arrows as a postprocessing option.

COMSOL Multiphysics Implementation—High-Accuracy Flux Computation

You will find that the flux calculated as outlined above does not match the expected pumping rate. This discrepancy results from using a low-density mesh. You might try to a achieve a high-accuracy flux by zooming in on the region of interest with finer elements. However, that reasoning applied to the tiny perforations amounts to a good formula for a bad hit in needless computational cost.

You often can get a high-accuracy flux and save on computation time using the Lagrange multipliers μ that COMSOL Multiphysics generates through an integral or weak PDE form. The Lagrange multiplier takes on the value of the flux at boundaries with strong constraints that assign the same pressure everywhere along the perforation edges. To access the Lagrange multipliers in this problem, use the non-ideal weak constraints at the boundaries of the perforations. With the weak constraints, the boundary pressure integral over the element is constrained, rather than pointwise in the Lagrange points. Furthermore, a high accuracy flux can be accessed at the element boundary. Now you can calculate the flux with the boundary integration described above, except that you replace the normal equation for a boundary flux with the Lagrange multiplier μ. To find out more, see "Computing Accurate Fluxes" on page 253 of the *COMSOL Multiphysics User's Guide*.

Data

The data used in this model are as follows:

VARIABLE	UNITS	DESCRIPTION	VAN GENUCHTEN
g_r	m/s^2	Gravity	9.82
ρ_f	kg/m^3	Fluid density	900
η_f	Pa·s	Dynamic viscosity	0.002
κ	m^2	Permeability	10^{-11}
θ_s		Porosity/void fraction	0.2
h_{well}	m	Thickness of reservoir	0.3048
r_{res}	m	Reservoir radius	6.5722
r_w	m	Well radius	0.1095

VARIABLE	UNITS	DESCRIPTION	VAN GENUCHTEN
W	m^3/s	Pumping rate	0.001
p_{well}	Pa	Pressure at perforations	10^5

Results

Figure 2-15 shows the solution for oil flow to a well centered at the origin. From this view, the pressure distribution and velocity field appear uniform. Note that the velocity is almost constant in the far field.

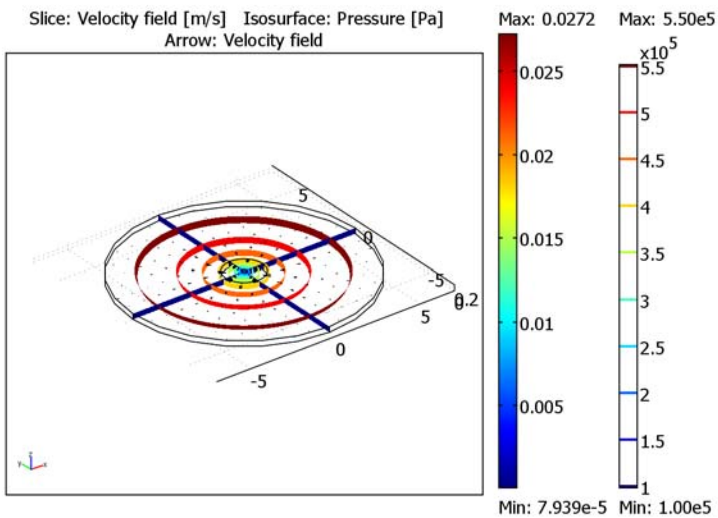


Figure 2-15: COMSOL Multiphysics solution of Darcy flow to a perforated wellbore: pressure (isosurface), velocity field (slice), and velocities (arrows).

Figure 2-16 gives a close-up view of the velocity field (wire-mesh isosurfaces) and pressure distribution (slice) immediately around the perforations in the well. The velocity results in Figure 2-16 are clearly nonuniform. The flow funnels to the perforations produce an antisymmetric swirl over the length of the wellbore. Comparing the pressure estimates in Figure 2-16 with those in Figure 2-15 indicates that the nonuniformity produced by the perforations covers a relatively small section of the flow field.

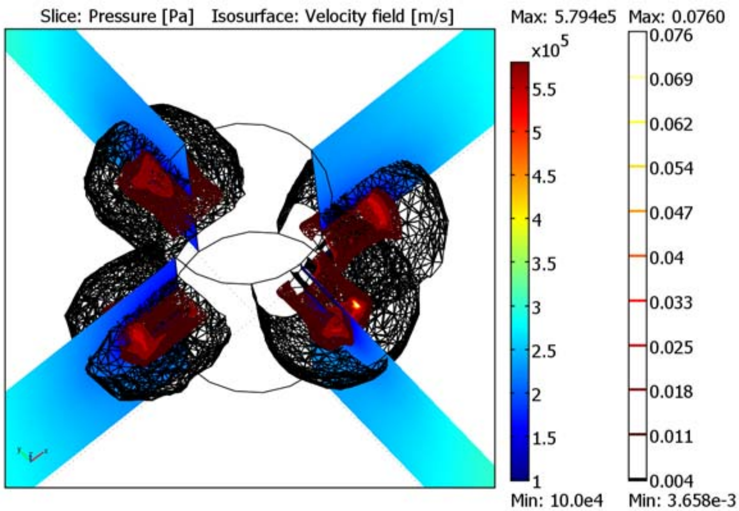


Figure 2-16: Close-up view of flow to a perforated wellbore: pressure (slices) and velocity field (wire-mesh isosurface).

To evaluate the accuracy of the simulation, compare the total flux through the perforations with the known pumping rate of 0.001 m^3/s. With the relatively coarse mesh (still with 40,000 elements), ordinary boundary integration gives a flux of 0.0014 m^3/s. A calculation in COMSOL Multiphysics with Lagrange multipliers, however, gives a flux of 0.00102 m^3/s. Adding the Lagrange multipliers improves the accuracy of the calculation to within 0.01% of the known pumping rate without increasing computational overhead.

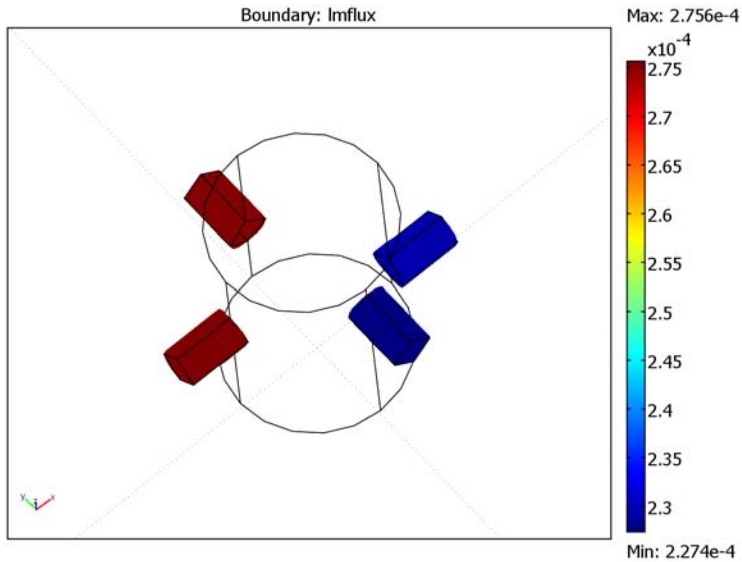


Figure 2-17: Estimates of fluid flux to perforations in a wellbore.

Figure 2-17 depicts the flux to individual perforations. With this geometry and orientation, a given perforation withdraws anywhere from 22% to 28% of the total pumping. The perforations closest to the impermeable confining units (above and below) withdraw significantly less fluid from the reservoir than those near the horizontal center line of the producing layer. This leads to the economically significant conclusion that changes in the orientation change the producing capability of a perforation by 6%.

References

1. A. Behie and A. Settari A, "Perforation Design Models for Heterogeneous Multiphase Flow," SPE Rocky Mountain Regional/Low Permeability Reservoir Symp., Denver, Colorado, paper 25901, pp. 591–602, 1993.

2. M. Jamiolahmady, A. Danesh, D.H. Terhani, G.D. Henderson, and D.B. Duncan, "Flow around a rock perforation surrounded by damaged zone: Experiments vs. Theory," IASME/WSEAS Int'l Conf., Corfu, Greece, 2004.

3. M. Muskat, “The effect of casing perforations on well productivity,” *Petroleum Trans. AIME*, vol. 151, pp. 175–187, 1943.

Model Library path: `Earth_Science_Module/Fluid_Flow/perforated_well`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**, and from the **Space dimension** list select **3D**.

2 From the list of application modes select **Earth Science Module>Fluid Flow>Darcy’s Law>Pressure analysis**.

3 Click **OK**.

GEOMETRY MODELING

1 Draw three cylinders by going to the **Draw** menu, selecting **Cylinder** and entering these settings:

NAME	CYL1	CYL2	CYL3
Radius	6.5722	1.0954	0.1095
Height	0.3048	0.3048	0.3048

2 Draw four small cylinders using the following data:

NAME	CYL4	CYL5	CYL6	CYL7
Radius	0.0254	0.0254	0.0254	0.0254
Height	0.1857	0.1857	0.1857	0.1857
Axis base point	[0 0 0.0381]	[-0.1857 0 0.1905]	[0 0 0.1143]	[0 -0.1857 0.2667]
Axis direction vector	[1 0 0]	[1 0 0]	[0 1 0]	[0 1 0]

3 Go to the Draw toolbar on the left side of the user interface and click the **Create Composite Object** button.

4 In the **Set formula** edit field enter the following expression: `CYL1+CYL2-(CYL3+CYL4+CYL5+CYL6+CYL7)`; when done, Click **OK**.

OPTIONS AND SETTINGS

1 From the **Physics** menu select **Scalar Variables**.

2 In the resulting dialog box enter the following names and expressions.

NAME	EXPRESSION
g_esdl	9.82
D_esdl	z

3 From the **Options** menu open the **Constants** dialog box.

4 Enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
p_well	100[kPa]	Pressure at perforations
W	0.001[m^3/s]	Pumping rate
r_res	6.5722[m]	Reservoir radius
h_well	0.3048[m]	Thickness of reservoir
k_int	1e-11[m^2]	Permeability
eta	0.002[Pa*s]	Dynamic viscosity
rho_f	900[kg/m^3]	Fluid density
r_well	0.1095[m]	Well radius

5 From the **Options** menu select **Integration Coupling Variables>Boundary Variables**. In the dialog box, create these boundary integration coupling variables, each on a separate row in the table; when done, click **OK**.

SOURCE BOUNDARY SELECTION	NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
9–13, 16–21, 24, 25, 28, 29, 32-36	flux	abs(flux_esdl)	4	yes
16–18, 24, 25	lmflux1	abs(lm1)	4	yes
9–13	lmflux2	abs(lm1)	4	yes
19–21, 28, 29	lmflux3	abs(lm1)	4	yes
32–36	lmflux4	abs(lm1)	4	yes

PHYSICS SETTINGS

Application Mode Properties

1 From the **Physics** menu, select **Properties**.

2 Select **On** in the **Weak constraints** list and **Non-ideal** in the **Constraint type** list, then click **OK**.

Subdomain Settings

1 Choose **Physics>Subdomain Settings**.

2 Select all active subdomains. In the **Storage term** list change **Specific storage** to **User defined**.

3 Enter the following material properties; when done, click **OK**.

VARIABLE	SUBDOMAINS 1, 2
S	`0`
K_s	`k_int`
ρ_f	`rho_f`
η	`eta`
Q_s	`0`

Boundary Conditions

From the **Physics** menu, open the **Boundary Settings** dialog box, then enter the following settings; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 2, 22, 31	BOUNDARIES 9–13, 16–21, 24, 25, 28, 29, 32–36	ALL OTHERS
Type	Inward flux	Pressure	Zero flux/Symmetry
N_0	`W/(2*pi*r_res*h_well)`	-	-
p_0	-	`p_well`	-

MESH GENERATION

1 From the **Mesh** menu, open the **Free Mesh Parameters** dialog box.

2 In the **Predefined mesh sizes** list select **Fine**.

3 Click the **Subdomain** tab.

4 In the **Subdomain selection** list choose **2**.

5 Set the **Maximum element size** to `0.01`, then click **OK**.

6 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 From the **Solve** menu, open the **Solver Parameters** dialog box.

2 The default solver cannot handle the weak constraints. Therefore go to the **Linear system solver** list and select **GMRES**, then go to the **Preconditioner** list and select **Incomplete LU**. Click **OK**.
3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To create Figure 2-15 on page 45, follow these steps:

1 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.
2 On the **General** page, go to the **Plot type** area and select the check boxes for **Slice**, **Isosurface**, and **Arrow**.
3 Click the **Isosurface** tab. On the **Isosurface Data** page, choose **Pressure** from the **Predefined quantities** list. Go to the **Isosurface levels** area, click the **Vector with isolevels** option button, and in the corresponding edit field enter `5e4:5e4:5.5e5`.
4 Click the **Slice** tab. In the **Slice data** area, select **Velocity field** from the **Predefined quantities** list. In the **Slice positioning** area, in both the **x levels** and **y levels** edit fields enter `1`, and in the **z levels** edit field enter `0`.
5 Click the **Arrow** tab. On the **Subdomain Data** page, select **Velocity field** from the **Predefined quantities** list. In the **Arrow positioning** area, in both the **x points** and **y points** edit fields enter `15`, and in the **z points** edit field enter `1`.
6 In the **Arrow parameters** area, click the **Color** button. In the **Arrow Color** dialog box, select black, then click **OK**.
7 Clear the **Auto** check box for the **Scale factor** and in the associated edit field type `0.5`.
8 Click **OK**.

To create Figure 2-16 on page 46, follow these steps:

1 From the **Postprocessing** menu open the **Plot Parameters** dialog box.
2 Go to the **General page**, and in the **Plot type** area clear the **Arrow** check box.
3 Click the **Isosurface** tab. On the **Isosurface Data** page, change the selection in the **Predefined quantities** list to **Velocity field**.
4 In the **Isosurface levels** area, click the **Number of levels** option button, then type `30` in the associated edit field.
5 In the **Coloring and fill** area, select **Wireframe** from the **Fill style** list.
6 In the **Isosurface color** area, select **hot** from the **Colormap** list.
7 On the **Slice** page, change the selection in the **Predefined quantities** list to **Pressure**.
8 Click **OK**.

9 Click the **Zoom In** button on the Main toolbar five times to zoom in on the wellbore. Click and drag in the drawing area to adjust the view.

To create Figure 2-17 on page 47, follow these steps:

1 Go to **Options>Expressions>Boundary Expressions** and define a boundary expression variable, `lmflux`, according to:

BOUNDARY SELECTION	NAME	EXPRESSION
16–18, 24, 25	`lmflux`	`lmflux1`
9–13	`lmflux`	`lmflux2`
19–21, 28, 29	`lmflux`	`lmflux3`
32–36	`lmflux`	`lmflux4`

2 From the **Solve** menu select **Update Model** to update the model with the new expression variable.

3 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.

4 On the **General** page, go to the **Plot type** area and select the check boxes for **Boundary** and **Geometry edges**.

5 Click the **Boundary** tab. In the **Expression** edit field, type `p`.

6 In the **Boundary color** area, select **hot** from the **Colormap** list.

7 Click **OK**.

Coupled Flow Laws

Understanding what happens during the transition from slow flow in porous media to fast flow in a channel is critical in many environmental cases and applied questions. This type of flow appears near rivers, estuaries, wellbores, caverns, and lava tubes, to name a few.

Traditionally, the quantitative assessment of transitioning flows has been the domain of those with time and tools to work out their own code because it requires switching between mathematical expressions for different flow laws. Darcy's law describes slow flow at a distance from the channel; the Navier-Stokes equations govern free or open-channel flows; and in between, where the fluid moves in porous media but shear is nonnegligible, the Brinkman or Forcheimer equations apply. This example demonstrates how to model such a transition using predefined equations in the Earth Science Module.

The following model examines transitioning flow by zooming in on oil movement to and within a perforated well. The analysis begins by coupling Darcy's law and the Brinkman equations to represent flow in porous media that quickens toward a perforation in the well casing. Next, it examines fluid movement into and within the well by coupling the Navier-Stokes equations to the Darcy-Brinkman model. Albeit counterintuitive, time-dependent Brinkman and Navier-Stokes are well known to be relatively easy to solve. This model instead analyzes a steady-state system.

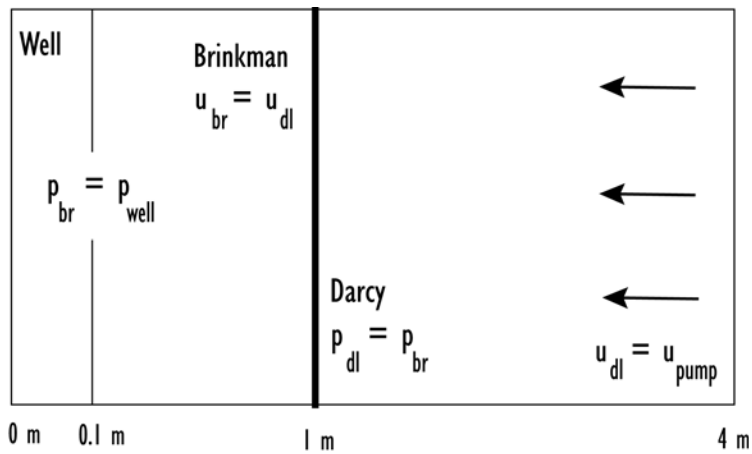


Figure 2-18: Model geometry showing boundary conditions for coupling Darcy's law (1 m < r < 4 m) and the Brinkman equations (0.1 m < r < 1 m).

By giving you the ability to link flow laws, modify predefined equations, and even freely define your own governing equations, COMSOL Multiphysics sees abundant use in analyzing conventional, coupled, and nonconventional flows (see Ref. 1 and Ref. 2).

Darcy-Brinkman: Model Definition

This Darcy-Brinkman example begins by overviewing the model setup and continues with the equations and the boundary conditions used in the analysis. Implementation details follow the mathematical background. The model triggers weak variables to implement the coupling between Darcy's law and the Brinkman equations. Finally this discussion reviews results and outlines the mechanics for building the model. The next example (Transitional Flow: Darcy-Brinkman–Navier-Stokes on page 69) adds the Navier-Stokes equations directly on top of the Darcy–Brinkman model file.

First examine a general description of the Darcy–Brinkman model. Oil moves through a thin porous layer towards a perforation to a well. The fluid flow follows Darcy's law in the far field (that is, 1 m < x < 4 m) and the Brinkman equations near the well opening (between 0.1 m < x < 1 m). The layer is 0.875 m thick and bounded above and below by impermeable materials that confine the permeable reservoir layer. For simplicity, assume the layer has homogeneous and isotropic hydraulic properties, and the fluid has constant density and viscosity. You know the flux of fluid at the inlet and the pressure at the perforations. The flow field is steady state.

Darcy's Law

Darcy's law describes fluid flow driven by gradients in pressure and elevation potential. The dependent variable in Darcy's law is pressure, p. The flows are slow enough that velocity head is negligible. For a steady state, the governing equation is

$$\nabla \cdot \left[-\frac{\kappa}{\eta}\nabla(p_{\mathrm{dl}} + \rho_{\mathrm{f}} g D)\right] = Q_s \,.$$

In this equation, κ denotes the permeability (m^2), η is the dynamic viscosity (kg/(m·s)), ρ_{f} gives the fluid density ($\mathrm{kg/m}^3$), and g the acceleration of gravity. Further, D is the coordinate for vertical elevation, and Q_s is the volumetric flow rate per unit volume of reservoir for a fluid source (1/s). You set D to zero in this problem because elevation potential is negligible given that the flow field is very thin. Because this model deals with multiple flow laws, this equation appends the "dl" subscript to p to denote the Darcy's law equation.

With a steady state, flow into the reservoir study area must equal the pumping rate. The Darcy velocity gives the inlet condition as

$$\mathbf{u}_{\mathrm{dl}} = -\frac{\kappa}{\eta}\nabla p_{\mathrm{dl}} = \frac{W}{2\pi r_{\mathrm{res}} b}$$

where W is the volumetric pumping rate for the perforated interval ($1/(\mathrm{m}^3 \cdot \mathrm{s})$), r_{res} equals the reservoir radius, and b is the reservoir thickness.

For a continuous solution across the interface between the zones of Darcy and Brinkman flow, the pressure and velocities from Darcy's law must equal the pressure and velocities from the Brinkman equations. Because a Neumann statement on flux already defines the inlet boundary, use the following constraint on pressure for the Darcy–Brinkman interface:

$$p_{\mathrm{dl}} = p_{\mathrm{br}} \,.$$

In this equation, the subscript "br" denotes the Brinkman equations. This expression is a Dirichlet boundary statement.

With no flow through the confining units that overlie and underlie the permeable reservoir zone, the boundary conditions for Darcy's law are

$$\mathbf{n} \cdot \left[\frac{\kappa}{\eta}(\nabla p_{\mathrm{dl}})\right] = -\frac{W}{2\pi r_{\mathrm{res}} b} \qquad \partial\Omega \quad \text{Inlet}$$

$$p_{\mathrm{dl}} = p_{\mathrm{br}} \qquad \partial\Omega \quad \text{Darcy-Brinkman interface}$$

$$\mathbf{n} \cdot \left[\frac{\kappa}{\eta}(\nabla p_{\mathrm{dl}})\right] = 0 \qquad \partial\Omega \quad \text{Confining layers}$$

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

Brinkman Equations

The Brinkman equations describe fluid flow in porous media where velocities are high enough that momentum transport by shear stress is important. Brinkman problems combine a momentum balance in the r and z directions with the continuity equation, giving dependent variables of directional velocities u and v as well as the pressure p. The Brinkman equations for steady state flow are

$$\begin{aligned} \left(-\nabla \cdot \frac{\eta}{\varepsilon}(\nabla \mathbf{u}_{\mathrm{br}} + (\nabla \mathbf{u}_{\mathrm{br}})^T)\right) - \left(\frac{\eta}{k}\mathbf{u}_{\mathrm{br}} + \nabla p_{\mathrm{br}} - \mathbf{F}\right) = 0 \\ \nabla \cdot \mathbf{u}_{\mathrm{br}} = 0 \end{aligned} \tag{2-1}$$

where ρ is density (kg/m^3), η gives the viscosity (kg/(m·s)) $\mathbf{u}$ equals the velocity vector (m/s), p is pressure (kg/(m·s)), ε is the porosity, and k (m/s) denotes the permeability. The equation can account for the influence of small gravity and compressibility effects in the force term, $\mathbf{F}$, which in this example equals zero. Some argue that k in the Brinkman equations differs slightly from κ in Darcy's law (Ref. 2), but this example calls for the same permeability in both flow zones.

From the Brinkman side of the Darcy–Brinkman interface you constrain velocity because the boundary condition on the Darcy side fixes the pressure. The velocity constraint on the Brinkman side of the interface reflects that velocities are dependent variables in the Brinkman equations but not in Darcy's law. The boundary condition on velocities is

$$\mathbf{u}_{\mathrm{br}} = \mathbf{u}_{\mathrm{dl}} \cdot$$

To implement the condition, use the Darcy velocities, $\mathbf{u}_{\mathrm{dl}}$, that COMSOL Multiphysics automatically calculates.

The confining layer and well casing are impermeable to flow. Approximate this situation with the no-slip condition

$$\mathbf{u}_{\mathrm{br}} = \mathbf{0}\,.$$

This equation eliminates all components of the velocity vector at the boundary.

Getting a unique solution to this problem requires defining the pressure at the well because the model prescribes flux conditions for all other boundaries. The constraint on pressure is the simple statement that

$$p_{\mathrm{br}} = p_{\mathrm{well}}\,.$$

For the Brinkman problem, the boundary conditions are now

$$\begin{array}{lll} \mathbf{u}_{\mathrm{br}} = \mathbf{u}_{\mathrm{dl}} & \partial\Omega & \text{Darcy-Brinkman interface} \\ \mathbf{u}_{\mathrm{br}} = \mathbf{0} & \partial\Omega & \text{Confining layers} \\ \mathbf{u}_{\mathrm{br}} = \mathbf{0} & \partial\Omega & \text{Well casing} \\ p_{\mathrm{br}} = p_{\mathrm{well}} & \partial\Omega & \text{Perforation.} \end{array}$$

Implementation—Coupling with Weak Constraints

The two equations in this analysis are fundamentally compatible as both describe fluid flow, pressure distributions, and velocities. Even so, the dependent variable in Darcy's law is pressure alone, whereas pressure and directional velocities are the dependent variables in the Brinkman equations. The difference in the number of dependent variables amounts to a slight incompatibility in form, which you circumvent by adding so-called non-ideal weak constraints on the equation system. The weak constraints provide new integral equations in which the Lagrange multipliers μ_1 are dependent variables. The constraints add one Lagrange multiplier to Darcy's law and two to the Brinkman equations to make up for the difference in the number of degrees of freedom given by the two governing equation systems on the boundaries. Adding the new Lagrange multipliers is easy—go to the **Application Mode Properties** dialog boxes, find the **Weak constraints** list, and select **On**. To make the weak constraints non-ideal, select **Non-ideal** from the **Constraint type** list.

To find out more about weak constraints and weak formulation equations, see "Using Weak Constraints" on page 300 in the *COMSOL Multiphysics Modeling Guide*.

Data

The data for parameterizing the model are:

VARIABLE	UNITS	DESCRIPTION	EXPRESSION
g_r	m/s^2	Acceleration due to gravity	9.82
ρ_f	kg/m^3	Fluid density	900
η_f	Pa·s	Dynamic viscosity	0.002
ε		Porosity	0.4
κ	m^2	Permeability	10^{-10}
b	m	Thickness of layer	1
r_{res}	m	Reservoir radius	4
r_w	m	Well radius	0.1
W	m^3/s	Pumping rate	10^{-3}
p_{well}	Pa	Pressure at perforation	105

Results

Figure 2-19 shows the solution to the Darcy-Brinkman problem where Darcy’s law governs slow flow far from the well, but near it the Brinkman equations apply. The impacts of the switch between flow laws occurs at $x = 1$ m. The streamlines show the fluid moving from the inlet at the right to the well on the left. The streamlines funnel because the flow is moving into a break or perforation in the well casing.

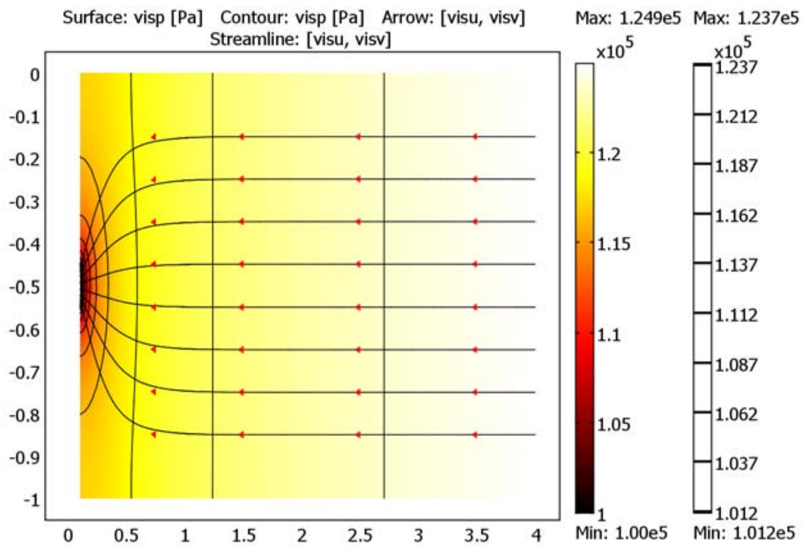


Figure 2-19: COMSOL Multiphysics solution for Darcy's law (1 m < r < 4 m) and the Brinkman equations (0.1 m < r < 1 m). The results shown are pressure (surface plot and contours) and velocities (streamlines). Note that the vertical axis is expanded.

Figure 2-20 and Figure 2-21, respectively, illustrate the pressure and velocity estimates from the perforation to a distance of 2 m beyond the Darcy-Brinkman interface.These estimates vary smoothly across the Brinkman-Darcy interface. Pressure increases with distance from the well, and it moves the fluid to the perforation. The velocities decrease with distance from the well until they reach an almost constant value in the Darcy flow zone. The fact that the pressure estimates vary smoothly from Brinkman (r < 1) to Darcy (r > 1) flow indicates a stable solution.

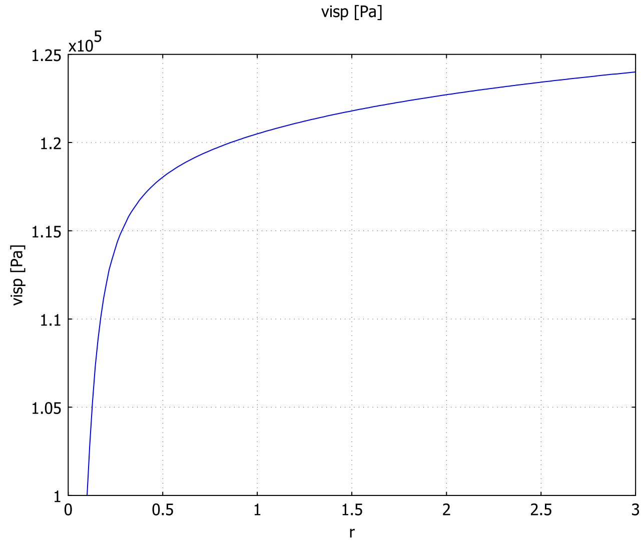


Figure 2-20: Pressure across the Darcy-Brinkman interface. Cross section along z = -0.5 m from r = 0.1 to 3.0 m.

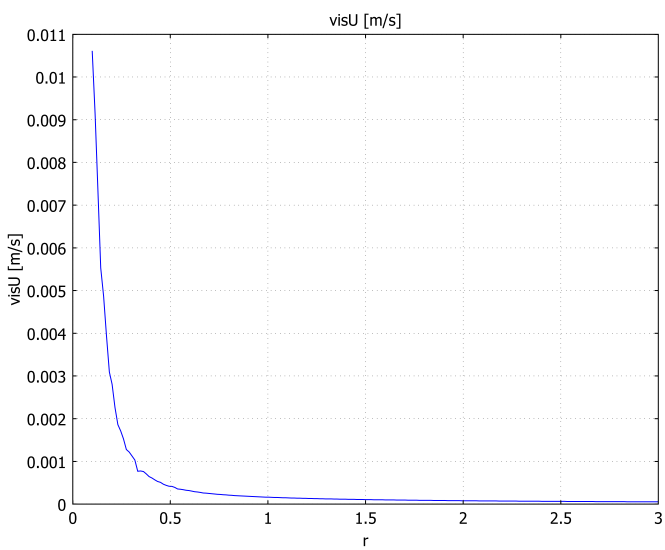


Figure 2-21: Velocity across the Darcy-Brinkman interface. Cross section along z = -0.5 m from r = 0.1 to 3.0 m.

This COMSOL Multiphysics example describes a straightforward protocol to couple two compatible flow laws with different dependent variables, the Darcy and Brinkman flow equations. Both Darcy's law and the Brinkman equations characterize flow in porous media. Because Darcy's law provides for no momentum transport by shear, it can overpredict flow rates in fast flow zones. Coupling to the Brinkman equations describes the added energy transformation.

The model is easy to modify and apply to a number of transitional flow scenarios including a river bottom, quickening flow near a well, and fluid moving in and around fractures. The next example adds the Navier-Stokes equations in the well to characterize the full transition between porous media and free surface flow.

References

1. M. Jamiolahmady, A. Danesh, D.H. Terhani, G.D. Henderson, and D.B. Duncan, "Flow around a rock perforation surrounded by damaged zone: Experiments vs. Theory," IASME/WSEAS Int'l Conf., Corfu, Greece, 2004.

2. U. Shavit, R. Rosenzweig, and S. Assouline, "Free flow at the interface of porous surfaces: A generalization of the Taylor Brush configuration," *Transport in Porous Media*, Kluwer Academic Publishers, 2003.

Model Library path: `Earth_Science_Module/Fluid_Flow/darcy_brinkman`

Modeling Using the Graphical User Interface

To begin the model, first add the Darcy's Law and the Brinkman equation application modes to the model file.

MODEL NAVIGATOR

1 Open the **Model Navigator**, and from the **Space dimension** list select **2D axisymmetry**.
2 In the list of application modes select **Earth Science Module>Fluid Flow>Darcy's Law>Pressure analysis>Steady-state analysis**.
3 In the **Application mode name** edit field change the name to `dl`. In the **Dependent variables** edit field enter `pdl`.
4 Click the **Multiphysics** button, then click **Add**. Keep the window open.

5 In the list of application modes select **Earth Science Module>Fluid Flow>Brinkman Equations**.

6 In the **Application mode name** edit field change the name to `chbr`. In the **Dependent variables** edit field enter `ubr vbr pbr`.

7 Click **Add**, then click **OK**.

GEOMETRY MODELING

Create the geometry by drawing three rectangles and adding a line at the perforation.

1 From the **Draw** menu select **Specify Objects>Rectangle**. In the dialog box, specify these settings for the rectangles; in each case, when done, click **OK**.

PARAMETER	R1	R2	R3
width	0.1	0.9	3
height	1	1	1
r	0	0.1	1
z	-1	-1	-1

2 Click the **Zoom Extents** button on the Main toolbar.

3 From the **Draw** menu select **Specify Objects>Line**. In the **Coordinates: r** edit field enter `0.1 0.1`; in the **Coordinates: z** edit field enter `-0.45 -0.55`.

4 Click **OK**.

OPTIONS AND SETTINGS

These variables reference the different solutions for each subdomain.

Select the menu item **Options>Constants** and enter these names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
pwell	1e5[Pa]	Pressure at perforation
W	1[l/s]	Pumping rate
b	1[m]	Layer thickness
perm	1e-10[m^2]	Permeability
eta	0.002[Pa*s]	Dynamic viscosity
rho	900[kg/m^3]	Fluid density
rres	4[m]	Reservoir radius

PHYSICS

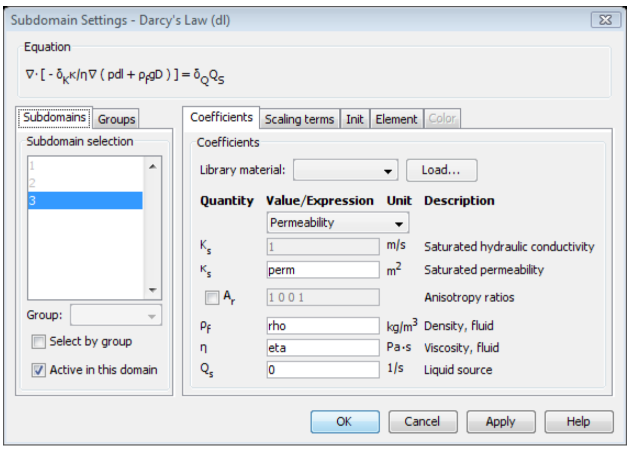
First set up the Darcy's Law application mode, then follow up with the Brinkman equations.

Darcy's Law Application Mode

1 In the **Multiphysics** menu select **Darcy's Law (dl)**.

2 Go to the menu item **Physics>Subdomain Settings**. Click the **Coefficients** tab. Deactivate the subdomain where the Brinkman equations apply; to do so, select Subdomains 1 and 2, then clear the **Active in this domain** check box.

3 Select Subdomain 3 and enter the settings from the following table in the user interface as shown.



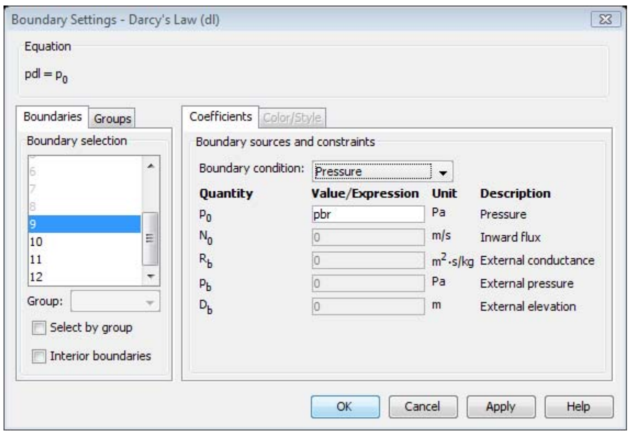
TERM	SUBDOMAIN 1
κ_s	`perm`
ρ_f	`rho`
η	`eta`

4 Click the **Init** tab. In the **Initial value** edit field enter `pwell`.

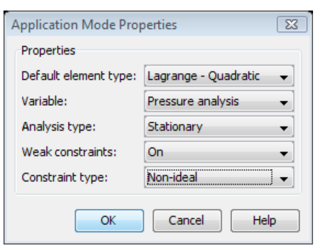
5 Click **OK**.

6 From the **Physics** menu choose **Boundary Settings**. Enter the settings from the following table; when done, click **OK**.

SETTINGS	BOUNDARY 9	BOUNDARY 12	BOUNDARIES 10, 11
Boundary condition	Pressure	Inward flux	Zero flux/Symmetry
p_0	`pbr`		
N_0		`W/(2*pi*rres*b)`	



7 From the **Physics** menu choose **Properties.** In the **Weak constraints** list select **On** and in the **Constraint type** list select **Non-ideal**; when done, click **OK**.



Brinkman Equations

1 In the **Multiphysics** menu select **Brinkman Equations (chbr)**.

2 Go to the menu item **Physics>Subdomain Settings**. Click the **Physics** tab. Deactivate the subdomain where Darcy's law and the Navier-Stokes equations applies; to do so, select Subdomains 1 and 3, then clear the **Active in this domain** check box.

3 Select Subdomain 2 and enter the following settings:

TERM	SUBDOMAIN 2
κ_s	`perm`
ε_p	`0.4`
η	`eta`
ρ_f	`rho`

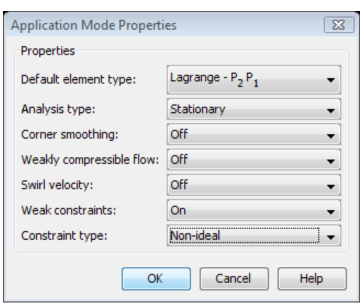
4 Click the **Init** tab. Enter the following settings; when done, click **OK**.

TERM	SUBDOMAIN 2
ubr	`W/(2*pi*r*b)`
vbr	`eps`
pbr	`pwell`

5 From the **Physics** menu choose **Boundary Settings**. Enter the following settings; when done, click **OK**.

SETTINGS	BOUNDARY 6	BOUNDARY 9	BOUNDARIES 4, 5, 7, 8
Boundary type	Outlet	Inlet	Wall
Boundary condition	Pressure, no viscous stress	Velocity	No slip
p0	`pwell`		
u		`u_dl`	
v		`v_dl`	

6 From the **Physics** menu choose **Properties.** In the **Weak constraints** list choose **On** and in the **Constraint type** list select **Non-ideal**. Click **OK**.



MESH GENERATION

The solution is sensitive to mesh size; the figures in this section arose from the following mesh setup.

1 From the **Mesh** menu select **Free Mesh Parameters**.
2 Click the **Subdomain** tab. Select Subdomain 2, then in the **Maximum element size** edit field enter `0.066`. Select Subdomain 3 and specify a **Maximum element size** of `0.133`.
3 Click the **Boundary** tab. Select Boundary 6 and in the **Maximum element size** edit field enter `0.005`. Select Boundary 9 and specify a **Maximum element size** of `0.02`.
4 Click **OK**.
5 Click the **Initialize Mesh** button on the Main toolbar.

   We generated the figures for this chapter by also clicking **Remesh**, but note that doing so adds significant computational effort to the simulation.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

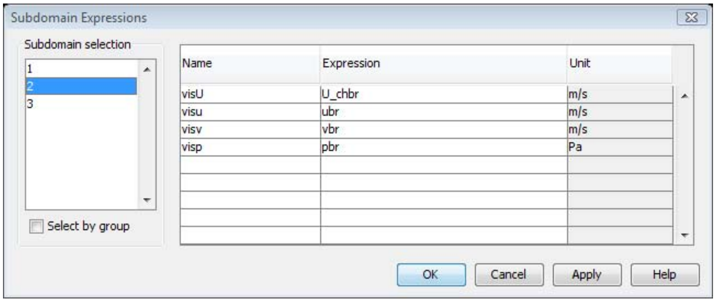
OPTIONS AND SETTINGS

A glance at the resulting figure indicates an incomplete view of the results—only those for Darcy's law appears. To view the solutions for both application modes at the same time, set up a few postprocessing variables that reference the different solutions for each subdomain.

1 Choose the menu item **Options>Expressions>Subdomain Expressions** and create the following expressions for Subdomains 2 and 3; when done, click **OK**.

NAME	SUBDOMAIN 2	SUBDOMAIN 3
`visU`	`U_chbr`	`U_dl`
`visu`	`ubr`	`u_dl`
`visv`	`vbr`	`v_dl`
`visp`	`pbr`	`pdl`

Here, `visU` displays the total velocity, `visu` displays the r-velocity, `visv` displays the z-velocity, and `visp` displays the pressure. As specified at the outset, the application mode name is `chbr` for the Brinkman equations and `dl` for Darcy's law. When you reference an application mode variable, you give the application mode name as a suffix. For example, because velocity is not a dependent variable in the Darcy's Law (dl) application mode but a variable COMSOL Multiphysics automatically creates for it, use the suffix `_dl` to reference it. You do not reference the application mode name to reference the pressure p_{dl} from Darcy's law because it is a dependent variable.



2 For the variables to take effect, you must update the model. From the **Solve** menu select **Update Model**.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 2-19 on page 59:

1 Select the menu item **Postprocessing>Plot Parameters**.

2 Click the **General** tab. In the **Plot type** area select the **Surface**, **Contour**, **Arrow**, and **Streamline** check boxes to activate those plots. Clear the **Geometry** check box.

3 Click the **Surface** tab. On the **Surface Data** page, enter `visp` in the **Expression** edit field, in the process typing over the current information in the edit field. Go to the **Surface color** area, and in the **Colormap** list select **hot**.

4 Click the **Contour** tab. On the **Contour Data** page, enter `visp` in the **Expression** edit field, also here typing over the current information. In the **Number of levels** edit field enter `20`. In the **Contour color** area click the **Uniform color** option button. Click the **Color** button, change the color to black, and then click **OK**.

5 Click the **Streamline** tab. On the **Streamline Data** page, type `visu` in the **r component** edit field and `visv` in the **z component** edit field.

6 Go to the **Start Points** page, click the **Specify start point coordinates** button. In the **r** edit field type `4 4 4 4 4 4 4 4`. In the **z** edit field enter `-0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15`.

7 Click the **Advanced** button. In the **Maximum number of integration steps** edit field type `10000`. In both the **Integration tolerance** and **Stationary point stop tolerance** edit fields type `0.00001`. Click **OK**.

8 Click the **Color** button. Select the color black, then click **OK**.

9 Click the **Arrow** tab. On the **Subdomain Data** page find the **r** edit field and enter `visu`, and in the **z** edit field enter `visv`.

10 In the **Arrow positioning** area click both **Vector with coordinates** option buttons. In the associated **r points** edit field, type
`3.5 3.5 3.5 3.5 3.5 3.5 3.5 3.5 2.5 2.5 2.5 2.5 2.5 2.5 2.5 2.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 0.75 0.75 0.75 0.75 0.75 0.75 0.75 0.75`.

11 In the corresponding **z points** edit field, type
`-0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15 -0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15 -0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15 -0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.35 -0.25`.

12 Go to the **Arrow parameters** area. In the **Arrow type** list select **cone**, and in the **Arrow length** list select **Normalized**. Click the **Color** button, choose the uniform color black, and then click **OK**. Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

To generate Figure 2-20 on page 60:

1 Select the menu item **Postprocessing>Cross-Section Plot Parameters**.

2 Click the **Line/Extrusion** tab. In the **y-axis data** area, type `visp` in the **Expression** edit field. In the **Cross-section line data** area, set **r0** to `0.1`, **r1** to `3.0`, and both **z0** and **z1** to `-0.5`. Click **Apply**.

To generate Figure 2-21 on page 60:

1 Still on the **Line/Extrusion** page of the **Cross-Section Plot Parameters** dialog box, change the **Expression** in the **y-axis data** area to `visU`. Click **OK**.

Transitional Flow: Darcy-Brinkman–Navier-Stokes

This example characterizes a transition in flow regimes: slow flow in porous media quickens to a perforation in a well casing and ultimately moves into and up the well. Darcy's law describes flow velocities at a distance from the well; closer to the perforation the Brinkman equations apply; the Navier-Stokes equations describe movement of fluid in the well. This example starts with a model that couples Darcy's law with the Brinkman equations. Adding the Navier-Stokes equations in the wellbore produces a fully coupled simulation for three different flow laws.

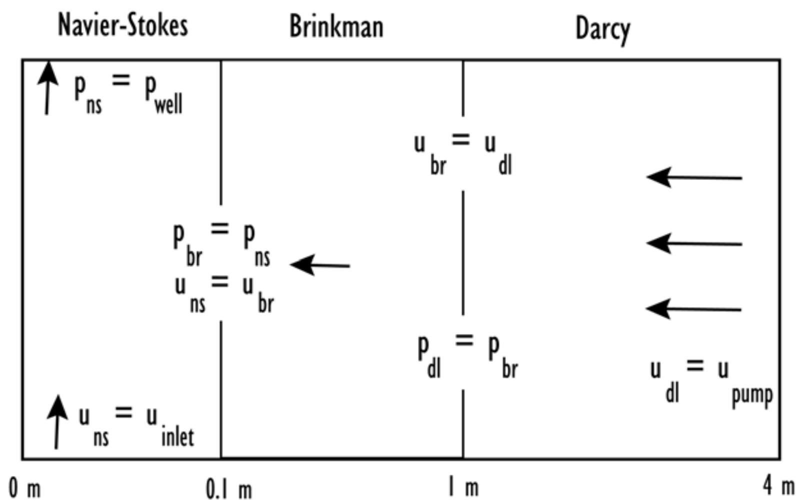


Figure 2-22: Geometry and boundary conditions used in COMSOL Multiphysics to couple the Darcy's law, Brinkman equations, and Navier-Stokes application modes.

The following pages describes the model. The first section reviews the Darcy, Brinkman, and Navier-Stokes equations and the boundary conditions. Next comes the solution procedure along with a data table. The final sections show results and gives step-by-step instructions for building the model in the COMSOL Multiphysics user interface.

Model Definition

Figure 2-22 illustrates the geometry and equation coupling in this example. Flow moves from $r = 4$ m within a permeable reservoir zone and exits to a well. The fluid entering the well combines with fluids moving upward from a permeable reservoir layer below the one in the model. In the study area, Darcy's law governs flow in the far field for $r > 1$ m. The Brinkman equations govern flow from the well casing at $0.1 \text{ m} < r < 1$ m. The interface between the Darcy and Brinkman flow zones occurs at $r = 1$ m. Within the well at $r < 0.1$ m the Navier-Stokes equations apply. The interface between the Brinkman and Navier-Stokes flow zones is the perforation at the midpoint of the casing. Otherwise there is no flow across the casing.

The problem setup for this example is identical to the Darcy–Brinkman model from the previous pages except for the boundary condition at the perforation and details inside the well. The model is 2D axisymmetry, covering a permeable zone 1 m deep over a reservoir radius of 4 m. The Darcy–Brinkman example specified that flow at $r = 4$ m satisfies the pumping rate and gives the pressure at the perforation. In this example, let COMSOL Multiphysics solve for the fluid pressure at the perforation and instead fix the pressure at the top of the well. The layer is homogeneous, isotropic, thin (specifically, 0.875 m), bounded above and below by impermeable materials, and the fluid has constant density and viscosity. You know the pumping rate and the pressure at the outlet, and you seek a steady-state solution to the flow field.

Darcy's Law

Darcy's law describes fluid flow in porous media driven by gradients in pressure alone. You can neglect elevation gradients in this problem because the flow field is very thin. For flow at steady state, the governing equation is

$$\nabla \cdot \left[-\frac{\kappa}{\eta} \nabla p_{\mathrm{dl}} \right] = Q_s$$

where κ is permeability (m^2), η equals the dynamic viscosity (kg/(m·s)), and Q_s is the volumetric flow rate per unit volume of reservoir for a fluid source (1/s).

The interface between the zones governed by Darcy's law and the Brinkman equations requires continuity in pressure and velocities. Because pressure is the dependent variable in Darcy's law, the boundary condition at the Darcy–Brinkman interface is a constraint on pressure,

$$p_{\mathrm{dl}} = p_{\mathrm{br}}$$

where the subscripts "dl" and "br" refer to Darcy's law and the Brinkman equations, respectively.

The remaining boundary conditions include a constraint on velocity at the reservoir inlet and at the impermeable confining layer. At the inlet, it is sufficient to satisfy the pumping rate. There is no flow across the confining layer. The boundary conditions for the Darcy's law problem are

$$
\begin{array}{ll}
\mathbf{n} \cdot \left[\dfrac{\kappa}{\eta}(\nabla p_{\mathrm{dl}})\right] = -\dfrac{W}{2\pi r_{\mathrm{res}} b} & \partial\Omega \;\; \text{Inlet} \\
p_{\mathrm{dl}} = p_{\mathrm{br}} & \partial\Omega \;\; \text{Darcy-Brinkman interface} \\
\mathbf{n} \cdot \left[\dfrac{\kappa}{\eta}(\nabla p_{\mathrm{dl}})\right] = 0 & \partial\Omega \;\; \text{Confining layer}
\end{array}
$$

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

Brinkman Equations

The Brinkman equations describe flow during the transition from Darcy to Navier-Stokes laws. With dependent variables of directional velocities and pressure, the Brinkman equations are

$$
\begin{gathered}
\left(-\nabla \cdot \frac{\eta}{\varepsilon}(\nabla \mathbf{u}_{\mathrm{br}} + (\nabla \mathbf{u}_{\mathrm{br}})^{T})\right) - \left(\frac{\eta}{\kappa}\mathbf{u}_{\mathrm{br}} + \nabla p_{\mathrm{br}}\right) = 0 \\
\nabla \cdot \mathbf{u}_{\mathrm{br}} = 0.
\end{gathered} \tag{2-2}
$$

In the equations, ρ denotes fluid density ($\mathrm{kg/m^3}$), η is viscosity ($\mathrm{kg/(m{\cdot}s)}$), $\mathbf{u}$ represents the velocity vector ($\mathrm{m/s}$), p is pressure ($\mathrm{kg/(m{\cdot}s)}$), ε is the porosity, and κ denotes the permeability ($\mathrm{m^2}$).

The Brinkman model constrains the velocity at the Darcy–Brinkman interface: the Brinkman velocity equals the Darcy velocity on the boundary. Except for the perforation, this example defines all other boundaries in the flow model with no-slip conditions, which is a statement about velocity. On the perforation, the model requires a condition that represents continuity in stress. The boundary conditions on the Brinkman flow zone are

$\mathbf{u}_{br} = \mathbf{u}_{dl}$	$\partial\Omega$	Darcy-Brinkman interface
$\mathbf{u}_{br} = \mathbf{0}$	$\partial\Omega$	Confining layers
$\mathbf{u}_{br} = \mathbf{0}$	$\partial\Omega$	Well casing
$(-p_{br}\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))\mathbf{n} = 0$	$\partial\Omega$	Perforation

Navier-Stokes Equations

The governing statement for flow in the wellbore comes from the Navier-Stokes equations, which combine a momentum balance with an equation of continuity:

$$-\nabla\cdot\eta(\nabla\mathbf{u}_{ns} + (\nabla\mathbf{u}_{ns})^T) + \rho\mathbf{u}_{ns}\cdot\nabla\mathbf{u}_{ns} + \nabla p_{ns} = 0$$
$$\nabla\cdot\mathbf{u}_{ns} = 0.$$

The Navier-Stokes equations and the Brinkman equations solve for dependent variables $\mathbf{u}$ and p. The "ns" subscript denotes the Navier-Stokes equation.

From the Navier-Stokes model, the interface to the Brinkman flow zone is the constraint on velocity as in

$$\mathbf{u}_{ns} = \mathbf{u}_{br}.$$

This equation states that the velocity at the perforation just inside the well equals the velocity just outside of it. Linking the Navier-Stokes and Brinkman velocities completes a chain that interconnects three flow laws beginning at the Brinkman-Darcy interface. In the chain, pressures and velocities for coupled flow laws link on opposite sides of an interface.

The remaining boundaries in the Navier-Stokes problem are a series of constraints on velocity and pressure. Velocity in the well drops to zero at the well casing, which correspond to a no-slip condition. You also know the volume flow rate, W_{in}, into the base of the well, the lower inlet. The well's centerline is a symmetry condition. Finally, you know the pressure at the well's upper outlet. In summary,

$$
\begin{array}{lll}
\mathbf{u}_{\mathrm{ns}} = u_{\mathrm{br}} & \partial\Omega & \text{Perforations} \\
\mathbf{u} = \bar{0} & \partial\Omega & \text{Casing} \\
\mathbf{n} \cdot \mathbf{u} = \dfrac{W_{\mathrm{in}}}{\pi r_{\mathrm{well}^2}} & \partial\Omega & \text{Well inlet (lower)} \\
\mathbf{n} \cdot \mathbf{u} = 0 & \partial\Omega & \text{Well centerline} \\
p = p_{\mathrm{well}} & \partial\Omega & \text{Well outlet (upper)}
\end{array}
$$

Implementation: Navier-Stokes Initial Guess

Systems involving Navier-Stokes equations are notoriously sensitive to the initial guess, even for a steady-state flow model such as this one. In this example, the Darcy-Brinkman problem solves readily, but establishing a good initial conditions for the Navier-Stokes zone requires an extra measure. A series of dummy simulations with the parametric solver helps to obtain iteratively better guesses about the velocities and the pressures throughout the wellbore. The parameter that varies in the simulations is the fluid viscosity. You start with a viscosity several orders of magnitude higher than the true value and solve for decreasing viscosity values. You also can get a good initial guess for Navier-Stokes problems by varying velocity values with the parametric solver.

Implementation: Coupling with Weak Constraints

This model employs non-ideal weak constraints to facilitate the coupling of flow laws with different dependent variables. This manual provides a foundation on the use of non-ideal weak constraints in previous model description for the Darcy-Brinkman interface. Nonetheless, this section provides the following reminder.

This model couples three compatible flow laws with different dependent variables. In Darcy's law the dependent variable is pressure alone, whereas pressure and directional velocities are dependent variables in the Brinkman and Navier-Stokes equations. To make up for the slight incompatibility of the equation forms, add non-ideal weak constraints to the equation system. The weak constraints add Lagrange multipliers that equalize the degrees of freedom between the three equation systems. You activate the non-ideal weak constraints by clicking an option in the **Application Mode Properties** dialog boxes. For more information about weak constraints and weak formulation equations, see “Using Weak Constraints” on page 300 in the *COMSOL Multiphysics Modeling Guide*.

Data

The following table lists data used in this model:

VARIABLE	UNITS	DESCRIPTION	EXPRESSION
g_r	m/s^2	Acceleration due to gravity	9.82
ρ_f	kg/m^3	Fluid density	900
η_f	Pa·s	Dynamic viscosity	0.002
κ	m^2	Permeability	$1 \cdot 10^{-10}$
ε		Porosity	0.4
b	m	Thickness of layer	0.875
r_{res}	m	Reservoir radius	4
r_{well}	m	Well radius	0.1
W	m^3/s	Extraction rate from the modeled permeable zone	$1 \cdot 10^{-3}$
W_{in}	m^3/s	Pumpage from underlying reservoirs moving through lower well inlet	$1 \cdot 10^{-4}$
p_{well}	Pa	Pressure at well outlet	$1 \cdot 10^{5}$

Results

Figure 2-23 shows the solution to the model for flow that transitions from Darcy's law in the far field ($r > 1$ m), to the Brinkman equations in the intermediate zone (0.1 m < r <1 m), to the Navier-Stokes equation in the well ($r < 0.1$ m). The pressure distribution (surface plot and contours) and velocities (arrows and streamlines) vary smoothly with no disruption at either the Darcy–Brinkman interface ($r = 1$) or the

Brinkman-Navier-Stokes interface (r = 0.1 m). The streamlines show fluid moving through the perforation and up the well.

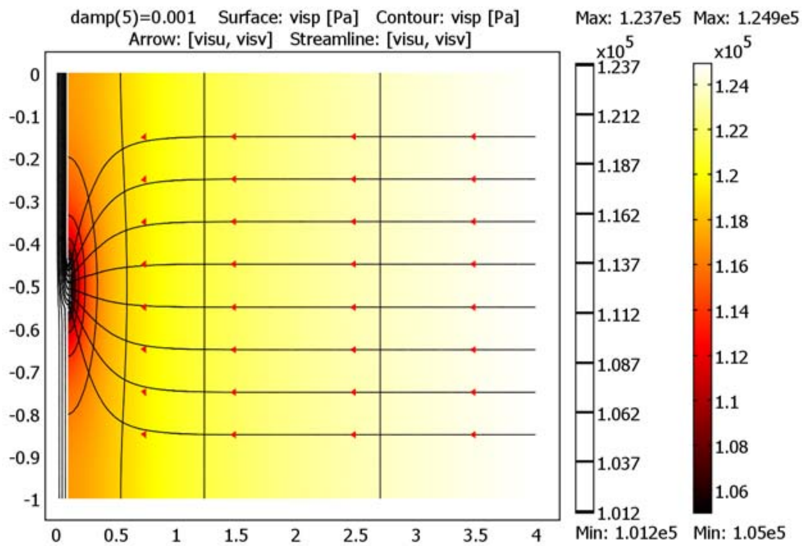


Figure 2-23: Distribution of pressure (surface plot and contours) and velocities (streamlines). Fluid flow follows Darcy's law (1 m < r < 4 m), the Brinkman equations (0.1 m < r < 1 m), and the Navier-Stokes equations (r < 0.1 m). The vertical axis is expanded for clarity.

In creating Figure 2-23 the author removed the pressure in the wellbore because it is almost uniform and disrupts the view of the streamlines. The small pressure drop in the well might seem disconcerting; however, it is reasonable and physically based. The well is an open channel. Within it a relatively small pressure drop can produce large volumetric flows because rocks do not impede fluid movement in the well.

Figure 2-24 is a close-up view of the velocity (surface plot) and pressure (contours) from the center of the well to r = 2 m. The figure covers the Navier-Stokes flow in the well, the Brinkman zone just beyond the well, and 1 m of the Darcy's law flow zone. Simulating the rapid velocity change in the well requires a good initial condition. In COMSOL Multiphysics you can obtain a good estimate for the distribution of starting velocities with a quick series of dummy simulations without the need to switch model files.

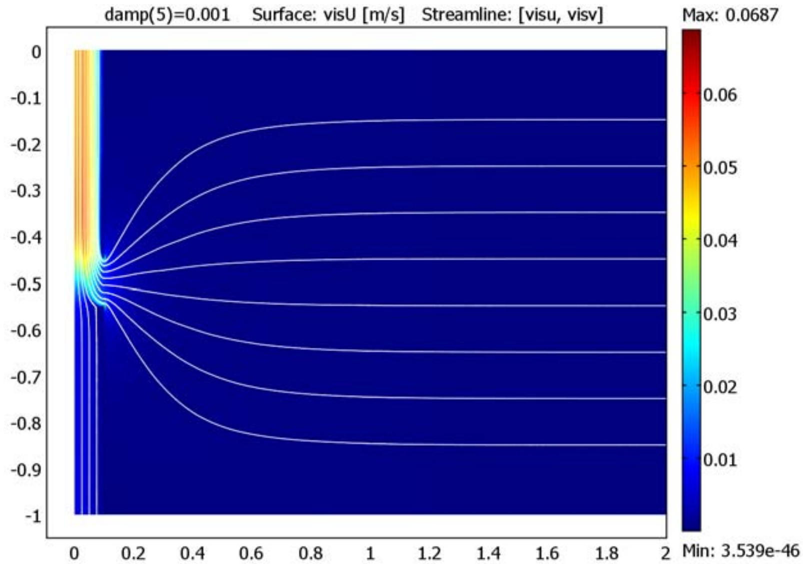


Figure 2-24: Close-up view of velocities (surface plot) and pressures (contours) within and near the wellbore. Fluid flow follows Darcy's law (1 m < r), the Brinkman equations (0.1 m < r < 1 m), and the Navier-Stokes equations (r < 0.1 m). The vertical axis is expanded for clarity.

Figure 2-25 shows the pressure along a cross section beginning in the well (Navier-Stokes) and ending a small distance beyond the well casing (Brinkman). The pressure is almost constant within the well because the flow in the well is vertical. The pressure rises smoothly beyond the Brinkman-Navier-Stokes interface. It is this pressure gradient that drives fluid into the well perforation.

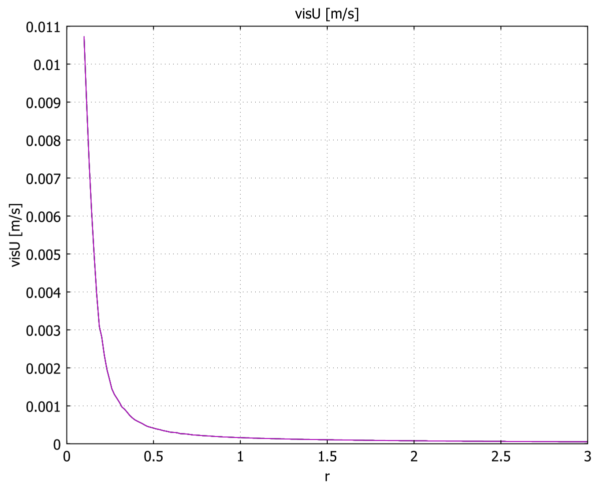


Figure 2-25: Pressure distribution at z = -0.5 m along the line r = 0.05 to 0.5 m.

Figure 2-26 provides a cross section of total velocity over the full transition between three different flow laws. It shows high velocities at the center of the well and no break in the profile at either the Brinkman-Navier-Stokes interface at r = 0.1 m or at the Darcy-Brinkman interface at r = 1 m.

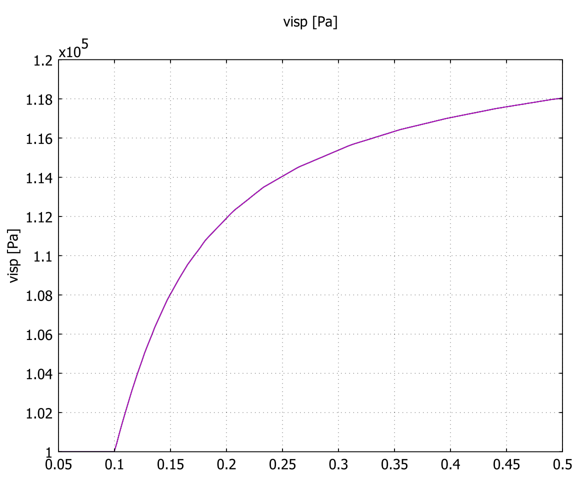


Figure 2-26: Velocity distribution at z = -0.5 m along the line r = 0.05 to 3.0 m.

This example demonstrates modeling of flows that transition through three different governing equations: the Navier-Stokes equations for free flow, the Brinkman equations for fast porous media flow, and Darcy's law for slow flow where you do not expect any energy dissipation by shear. This particular model describes the transitioning flow to a well, but the concept applies to many other environmental and applied scenarios including rivers, tubes, pipes, and springs. In the past, the transition between flow laws has often been the domain of academic research efforts because most off-the-shelf software packages focus on one flow type or another. COMSOL Multiphysics, though, can link together a number of different flow equations.

Model Library path: `Earth_Science_Module/Fluid_Flow/darcy_brinkman_ns`

Modeling Using the Graphical User Interface

To begin the model, first open the Darcy-Brinkman example and add the Navier-Stokes equations to the model file.

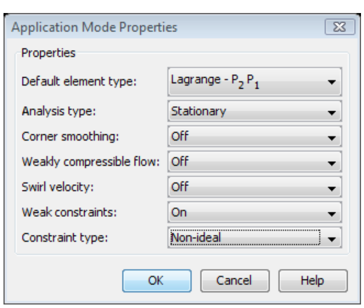
MODEL NAVIGATOR

1 Open the **Model Navigator** and click the **Model library** tab. From the model tree select **Earth Science Module>Fluid Flow>darcy brinkman**. Click **OK**.

2 After the model loads, go to the **Multiphysics** menu and select **Model Navigator**.

3 In the list of application modes select **Earth Science Module>Fluid Flow>Incompressible Navier-Stokes equations**. In the **Application mode name** edit field replace the existing text by entering `ns`, and in the **Dependent variables** edit field replace the existing text with `uns vns pns`. Click **Add**.

4 Click the **Application Mode Properties** button. Choose **On** in the **Weak constraints** list and **Non-ideal** in the **Constraint type** list. Click **OK**.



5 Click **OK** to close the **Model Navigator**.

APPLICATION SCALAR VARIABLES

There are no scalar variables to check with the Navier-Stokes application mode.

OPTIONS AND SETTINGS

1 Several variables reference the different solutions for each subdomain. To set them up, go to the menu item **Options>Constants**.

2 Enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rwell`	`0.1[m]`	`Well radius`
`Win`	`W/10`	`Pumpage from underlying reservoirs moving through lower well inlet`

3 For viewing the entire solution, add the Navier-Stokes results to the processing variables that already reference the Darcy's law and Brinkman results in corresponding subdomains. To do so, go to the menu item **Options>Expressions>Subdomain Expressions**. In the resulting dialog box enter the following expressions for the three subdomains; when done, click **OK**.

NAME	SUBDOMAIN 1	SUBDOMAIN 2	SUBDOMAIN 3
`visU`	`U_chns`	`U_chbr`	`U_dl`
`visu`	`uns`	`ubr`	`u_dl`
`visv`	`vns`	`vbr`	`v_dl`
`visp`	`pns`	`pbr`	`pdl`

In this table, `visU` describes total velocity, `visu` is the x-velocity, `visv` gives the y-velocity, and `visp` is the pressure. The application mode name is `chns` for the Navier-Stokes equations, `chbr` for the Brinkman equations, and `dl` for Darcy's law. No suffix is needed to reference the dependent variable in an equation. For calculated variables the application mode name is a suffix. For example, because velocity is not a dependent variable in the Darcy's law application mode but is a variable automatically created for it, reference it with the suffix `_dl`.

PHYSICS

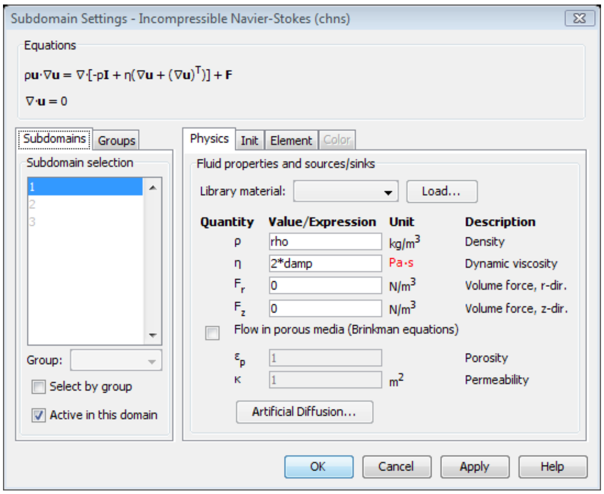
Set up the Navier-Stokes application mode and solve it for a dummy simulation.

Navier-Stokes Application Mode

1 From the **Physics** menu select **Subdomain Settings**.

2 Click the **Physics** tab. Deactivate the subdomains where the Brinkman equations apply; to do so, select Subdomains 2 and 3, then clear the **Active in this domain** check box.

3 Select Subdomain 1. In the η edit field for **Dynamic viscosity** enter `2*damp`, and in the ρ edit field for **Density** enter `rho`.



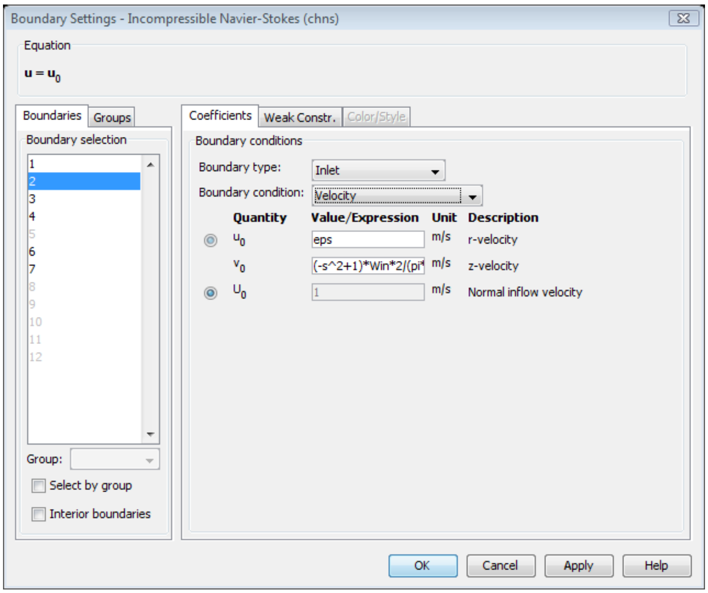
4 Click the **Init** tab. Enter the following settings; when done, click **OK**.

TERM	SUBDOMAIN 1
uns	`eps`
vns	`W/(pi*rwell^2)`
pns	`pwell`

5 From the **Physics** menu choose **Boundary Settings**. For the various boundaries enter the settings from the following table; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	BOUNDARY 6	BOUNDARIES 4, 7
Boundary type	Symmetry boundary	Inlet	Outlet	Inlet	Wall
Boundary condition	Axial symmetry	Velocity	Pressure, no viscous stress	Velocity	No slip
p_0			`pwell`		

SETTINGS	BOUNDARY 1	BOUNDARY 2	BOUNDARY 3	BOUNDARY 6	BOUNDARIES 4, 7
u_0		`eps`		`ubr`	
v_0		`(-s^2+1)*2*Win /(pi*rwell^2)`		`vbr`	



In the previous table, `s` is the arc length of a boundary, which goes from 0 at the start point to 1 at the end point. COMSOL Multiphysics denotes the end point with an arrow on the boundary. Use `s` to give a parabolic velocity profile at the well inlet.

Brinkman Equations

1 From the **Multiphysics** menu select **Brinkman Equations (chbr)**.

2 From the **Physics** menu select **Boundary Settings**. Select Boundary 6. Select the **Boundary type Outlet** and the **Boundary condition Pressure**. In the $\mathbf{p_0}$ edit field for **Pressure** enter `pns`. Click **OK**.

MESH GENERATION

1 From the **Mesh** menu select **Free Mesh Parameters**.

2 Click the **Subdomain** tab. Select Subdomain 1, then in the **Maximum element size** edit field enter `0.02`. Select Subdomain 2, then in the **Maximum element size** edit field enter `0.066`. Select Subdomain 3 and specify a **Maximum element size** of `0.133`.

3 Click the **Boundary** tab. Select Boundary 6 and in the **Maximum element size** edit field enter `0.005`. Select Boundary 9 and specify a **Maximum element size** of `0.02`.

4 Click the **Point** tab. Select Points 4 and 5, then in the **Maximum element size** edit field enter `0.001`. For **Growth rate** enter `1.1`.

5 Click **OK**.

6 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

To solve the model, first clear the old solution then iterate to solve the 3-way coupled problem.

1 Go to the **Solve** menu and return to the **Solver Parameters** dialog box. From the **Solver** list, click **Parametric**. For **Parameter name** enter `damp`. For **Parameter values** enter `0.1 0.01 0.005 0.0025 0.001`. Click **OK**.

2 Click the **Start** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 2-23 on page 75 follow these steps:

1 From the **Postprocessing** menu open the **Plot Parameters** dialog box.

2 Click the **General** tab. In the **Plot type** area click the **Surface**, **Contour**, and **Streamline** check boxes. Clear the **Geometry** check box.

3 Click the **Surface** tab. On the **Surface Data** page, enter `visp` in the **Expression** edit field, typing over the current information. In the **Surface color** area, find the **Colormap** list and select **hot**.

4 Click the **Contour** tab. On the **Contour Data** page, enter `visp` in the **Expression** edit field, again typing over current information. In the **Contour levels** area, enter `20` in the **Number of levels** edit field. Proceed to the **Contour color** area. Click first the **Uniform color** option button and then the **Color** button. Choose black, then click **OK**.

5 Click the **Streamline** tab. On the **Streamline Data** page, enter `visu` and `visv` in **r component** and **z component** edit fields, respectively. On the **Start Points** page, click the **Specify start point coordinates** option button. In the **r component** edit field enter `0.02 0.04 0.06 0.08 4 4 4 4 4 4 4 4`, and in the **z component** edit field enter `-1 -1 -1 -1 -0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15`. Click the **Advanced** button. In the **Maximum number of integration steps** edit field enter `10000`. In both the **Integration tolerance** and the **Stationary point stop tolerance** edit fields enter `0.00001`, then click **OK**. Click the **Color** button, set the color to black, and then click **OK**.

6 Click the **Arrow** tab. On the **Subdomain Data** page enter `visu` in the **r component** edit field and `visv` in the **z component** edit field. In the **Arrow positioning** area click both **Vector with coordinates** option buttons.

7 In the edit field associated with **r points** enter `3.5 3.5 3.5 3.5 3.5 3.5 3.5 3.5 2.5 2.5 2.5 2.5 2.5 2.5 2.5 2.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 0.75 0.75 0.75 0.75 0.75 0.75 0.75 0.75`.

8 In the edit field associated with **z points** enter `-0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15 -0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15 -0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.25 -0.15 -0.85 -0.75 -0.65 -0.55 -0.45 -0.35 -0.35 -0.25`.

9 In the **Arrow parameters** area find the **Arrow type** list and select **Cone**. In the **Arrow length** list select **Normalized**. Click the **Color** button, set the color to black, and then click **OK**.

10 Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

To generate Figure 2-24 on page 76, continue with these steps:

1 From the **Postprocessing** menu select **Plot Parameters**.

2 On the **General** page, clear the **Streamline** and **Arrow** check boxes.

3 Click the **Surface** tab. On the **Surface Data** page, enter `visU` in the **Expression** edit field, typing over the current information. Go to the **Surface color** area, and in the **Colormap** list choose **jet**.

4 Click the **Contour** tab. On the **Contour Data** page, enter `visp` in the **Expression** edit field, typing over the current information. In the **Contour levels** area, enter `10` in the **Number of levels** edit field. In the **Contour color** area, click first the **Uniform color** option button, then click the **Color** button. Change the color to white, then click **OK**.

5 Click **OK** to close the **Plot Parameters** dialog box.

6 Use the **Zoom Window** tool on the Main toolbar to zoom in on the area of interest.

To generate Figure 2-25 on page 77, continue with these steps:

1 Select the menu item **Postprocessing>Cross-Section Plot Parameters**.

2 Click the **Line/Extrusion** tab. In the **y-axis data** area, enter `visp` in the **Expression** edit field. In the **Cross-section line data** area, set **r0** to `0.05`, **r1** to `0.5`, and both **z0** and **z1** to `-0.5`. Click **Apply**.

To generate Figure 2-26 on page 77, continue with these steps:

3 In the **y-axis data** area, change the **Expression** to `visU`.

4 In the **Cross-section line data** area, change **r1** to `3.0`. Click **OK**.

Discrete Fracture—Porous Media Flow

Fluids in fractured porous media move quickly through the fractures but also migrate, albeit relatively slowly, through the tiny pores within the surrounding matrix blocks. Some fluid transfers between the fractures and the matrix blocks, so fluid pressures are continuous across the fracture from block to block. Accurately predicting fracture and matrix flow is often critical to assessing well productivity, to delineating migrating pollution, and to designing pollution cleanup strategies, to name just a few uses.

This example demonstrates a new efficient and accurate method to jointly model the fracture and matrix flows in a fractured block. You build it by representing the fractures as the boundaries between adjacent matrix blocks (Figure 2-27). Darcy's law governs velocities in the matrix blocks, while you set up flow in the fractures on boundaries by accounting for the fracture's thickness. Representing the fracture as an interior boundary is especially efficient because it eliminates the need to create a geometry with a high aspect ratio with a very long and narrow fracture domain that otherwise would require a dense mesh consisting of great number of tiny elements.

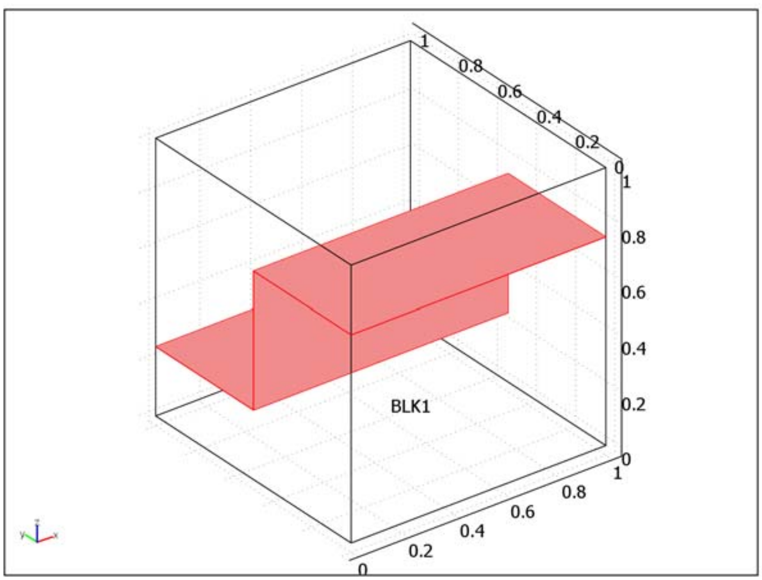


Figure 2-27: Geometry for a COMSOL Multiphysics analysis of a discrete fracture.

Model Definition

The geometry in Figure 2-27 is a block of fractured porous media that measures 1 m on each side. The fracture is far more permeable to fluid than the matrix block and has a thickness of 0.0001 m, which is much smaller than the block dimensions. Here the walls of the block are impermeable to flow except at the fracture edges, but such need not be the case. Fluid moves from left to right through the block entering at the lower fracture edge and exiting at the upper edge. The fluid initially does not move within the volume. Pressure at the outlet edge drops with time., while pressure at the inlet edge remains at the initial pressure throughout the simulation. The simulation period is 1000 s. At the end of this discussion a tabulation of the data values appears.

FLUID FLOW—MATRIX BLOCK

Time-dependent fluid flow in the matrix block is governed by Darcy's law

$$[\chi_f\theta_s + \chi_s(1-\theta_s)]\frac{\partial p}{\partial t} - \nabla \cdot \left[\frac{\kappa_m}{\eta}\nabla p\right] = 0 \qquad \Omega \text{ matrix block}$$

where the dependent variable, p, is the fluid's pressure in the pore space (kg/(m·s^2)), θ_s is the void fraction or porosity of the matrix blocks (m^3/m^3), χ_f and χ_p are the compressibilities of the fluid and solid (s^2·m/kg), respectively, κ_m gives the permeability of the matrix blocks (m^2), η equals the fluid's dynamic viscosity (Pa·s), and D is the vertical axis (m).

In the blocks, the predefined velocity variable, u_{esdl} (m/s), gives the Darcy velocity, which is a volume flow rate per unit area of porous media:

$$u_{esdl} = -\frac{\kappa_m}{\eta}\nabla p \qquad \Omega \text{ matrix block} \; .$$

The fluid's linear velocity within the small interstices in the block, u_{lin}, is higher than the Darcy velocity, which describes the velocity as if it were distributed over both solids and voids, $u_{lin} = u_{esdl}/\theta_s$.

Along all faces of the block the zero flow boundary condition applies:

$$\mathbf{n} \cdot -\frac{\kappa_m}{\eta}\nabla p = 0 \qquad \partial\Omega \text{ block face}$$

where $\mathbf{n}$ is the outward pointing normal to the boundary. This means that flow going perpendicular to and across the boundary equals zero.

FLUID FLOW—FRACTURE

The fracture in the model is a sequence of interior boundaries. Typically at a boundary you define flow across or normal to the boundary instead of along it. In this model, however, you employ special tangential options from COMSOL Multiphysics that allow for defining flow along the interior boundaries or fracture.

For this type of analysis to be valid, the equation on the fracture must solve for the same dependent variable as the equation for the matrix block, p. In this particular example, the equation for velocity in the fracture follows a modified form of that within the matrix block, namely Darcy's law. You modify the equation coefficients to account for a relatively small resistance to flow on the fracture and the fracture thickness, which gives dimensional consistency between the fracture and matrix:

$$S_{\mathrm{frac}}\frac{\partial p}{\partial t} - \nabla\cdot\left[\frac{\kappa_{\mathrm{frac}}}{\eta}d_{\mathrm{frac}}\nabla p\right] = 0 \qquad \partial\Omega \ \ \text{fracture} \ \cdot$$

In the equation, S_{frac} is the fracture-storage coefficient ($s^2\cdot m/kg$), κ_{frac} describes the fracture's permeability (m^2), and d_{frac} is the fracture's thickness (m).

Because thickness appears in the fracture flow equation, the predefined variable u_{esdl} now gives the volume flow rate per unit length of fracture:

$$u_{\mathrm{esdl}} = -\frac{\kappa_{\mathrm{frac}}}{\eta}d_{\mathrm{frac}}\nabla p \qquad \partial\Omega \ \ \text{fracture.}$$

The linear velocity of the fluid within the fracture is $u_{\mathrm{esdl}}/d_{\mathrm{frac}}$.

Bounding the fracture are edges that intersect the porous media block. The pressure is known at the inlet edge. At the outlet edge the flow rate u_{esdl} is known. There is no flow through the other edges.

$$\begin{aligned} p &= p_{\mathrm{inlet}} && \partial^2\Omega \ \ \text{inlet edge} \\ p &= p_{\mathrm{outlet}} && \partial^2\Omega \ \ \text{outlet edge} \\ -\frac{\kappa_{\mathrm{frac}}}{\eta}d_{\mathrm{frac}}\nabla p &= 0 && \partial^2\Omega \ \ \text{other edges.} \end{aligned}$$

Implementation

To trigger flow on the fracture that interacts with flow in the matrix, you add weak form equations with tangential derivatives on the interior boundaries. The weak PDE formulation is the extremely powerful and flexible integral form that underlies the finite element method. The tangential derivatives p_{Tx}, p_{Ty}, and p_{Tz} describe the change in pressure along, rather than across, the boundary. With weak PDEs, the time rate change in pressure goes into a `dweak` expression that combines with velocities and sources in `weak` expressions to completely describe the physics. To find out more about the use of the weak PDE form see “The Weak Form” on page 291 in the *COMSOL Multiphysics Modeling Guide*.

Results

The following figures contain screen shots from the analysis of time-dependent flow in a fractured porous media block. The isosurfaces in Figure 2-28 show the contours of fluid pressures throughout the block at the final output time of 1000 s. The pressures are continuous across the fracture from block to block. Even so, the bends in the isosurfaces indicate different flow regimes in the fracture and the matrix blocks. The arrows indicate velocities on the fracture. The fluid moves from inlet to the outlet along the fracture with a velocity field that is uniform across the block.

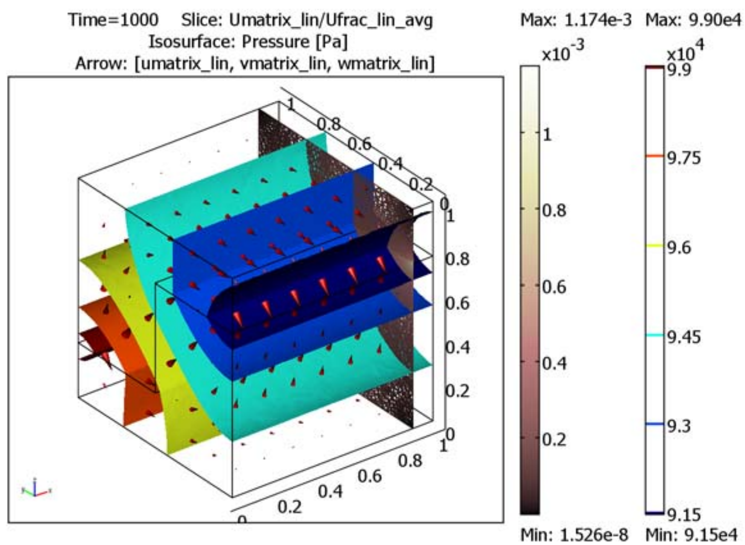


Figure 2-28: Results at time 1000 s for the analysis of flow in a porous media block with a fracture running through it: shown are the pressure (surface plot), linear velocity along the fracture (arrows), and maximum linear velocity (max/min). Pressure isosurfaces go from 91,500 to 100,000 Pa at 1500 Pa increments. The maximum velocity on the fracture is 1.13 m/s.

Figure 2-29 shows the linear velocities of the fluid in the matrix along with the pressure surface from Figure 2-28. With no flow out of the matrix, the only fluid source is the fracture. The arrows indicate that fluid exits from the fracture at the inlet. The matrix flow feeds the fracture at the outlet. The wireframe slice plot shows that the linear velocity in the matrix is orders of magnitude smaller than the average linear velocity along the fracture at time 1000 s.

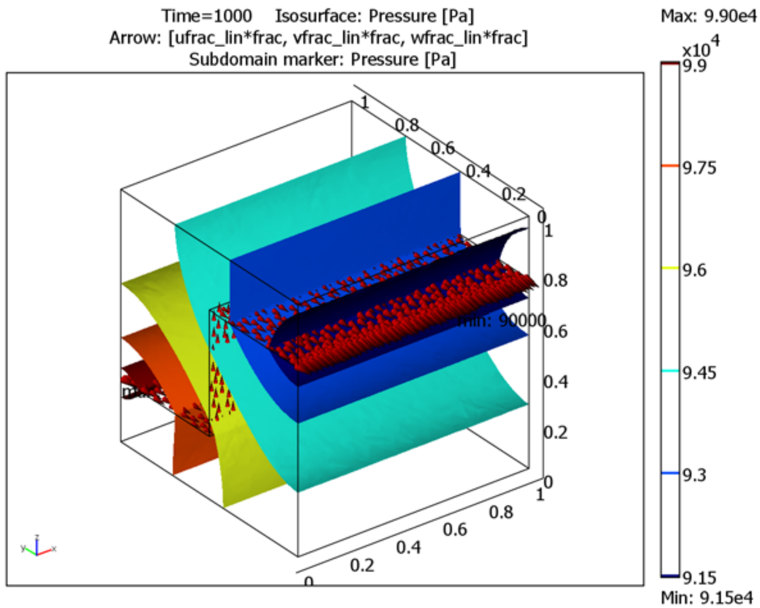


Figure 2-29: Results from the analysis of a porous media block with a discrete fracture; it shows fluid pressure (the isosurfaces), velocities in the matrix blocks (black arrows), and matrix linear velocity relative to average linear fracture velocity (slice plot).

Figure 2-30 illustrates the flow field in the fractured block evolving over the 1000 s simulation period. The isosurfaces stack up in the block as the pressure drop increases but stay centered on the fracture. At an early time, the matrix velocity and the fracture velocities differ by a factor of 1000. At a late time, the ratio between the linear velocities in the block and the velocities on the fracture are on the order of 1,000,000.

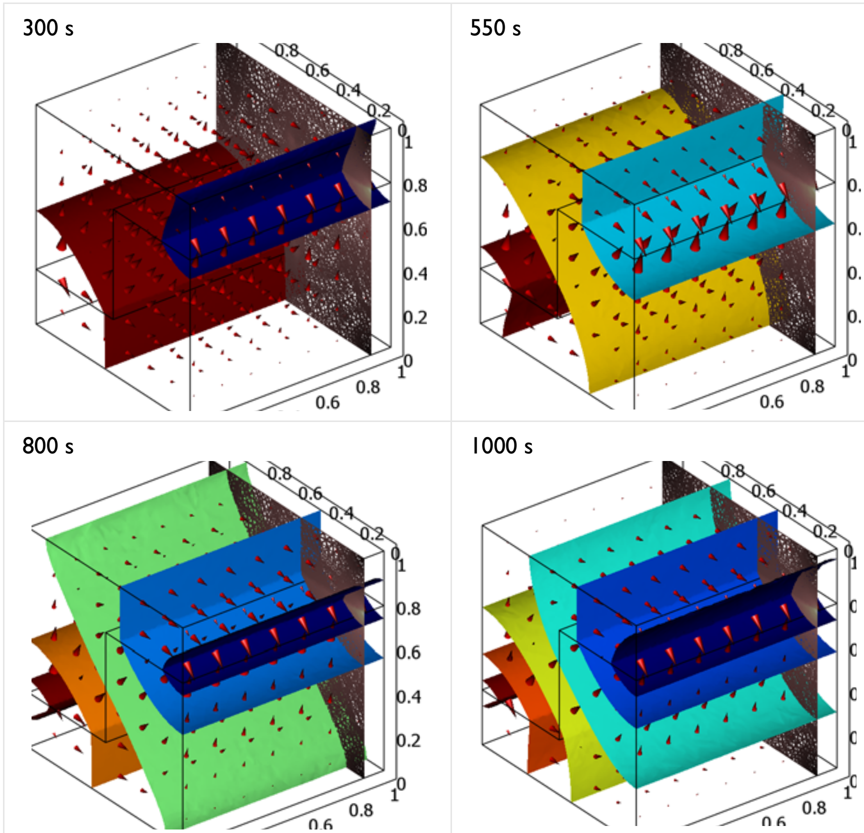


Figure 2-30: Postprocessing images from the analysis of flow on a discrete fracture in a matrix block. Shown are the fluid pressure (the isosurfaces), velocities in the matrix blocks (black arrows), and matrix linear velocity relative to average linear fracture velocity.

Conclusions

This example shows how to model flow in a discrete fracture that interacts with fluid flow in the porous matrix that surrounds it. The method used here is especially efficient computationally. With COMSOL Multiphysics' tangential boundary options, you can represent the fracture as a 2D boundary rather than a 3D model domain. This approach produces high-resolution results and also eliminates the need for an enormous number of small elements.

Data

The coefficients and parameters in this model are as follows:

VARIABLE	UNITS	DESCRIPTION	EXPRESSION
θ_s	m^3/m^3	Porosity of matrix blocks	0.3
χ_f	$s^2 \cdot m/kg$	Compressibility of the fluid	$4.4 \cdot 10^{-10}$
χ_s	$s^2 \cdot m/kg$	Compressibility of the fluid	10^{-8}
κ_m	$1/m^2$	Permeability of matrix blocks	10^{-11}
d_f	m	Thickness of the fracture	0.0001
S_f	$s^2 \cdot m/kg$	Storage coefficient of the fracture	χ_f
κ_f	$1/m^2$	Permeability of fracture	10^{-7}
η	kg/m·s	Viscosity	0.001
g_r	m/s^2	Gravity	9.82
ρ_f	kg/in^3	Fluid density	1000
p_{inlet}	$kg/m \cdot s^2$	Pressure at the fracture inlet	10^5
p_{outlet}	$kg/m \cdot s^2$	Pressure at the fracture outlet	$p_0 - 10t$
p_0	$kg/m \cdot s^2$	Initial pressure distribution	10^5

Model Library path: `Earth_Science_Module/Fluid_Flow/fracture`

Modeling Using the Graphical User Interface

In this example, the geometry already exists as a COMSOL Multiphysics model file. Ordinarily to build a 3D model you start with the following steps.

MODEL NAVIGATOR

1 Open the **Model Navigator**. In the **Space dimension** list select **3D**.

2 In the list of application modes choose **Earth Science Module>Fluid Flow>Darcy's Law>Pressure analysis>Transient analysis**.

3 Click **OK**.

SCALAR VARIABLES

Because of the small model domain you can neglect the impact of gravity, so there is no need to alter the settings available from the **Physics>Scalar Variables** dialog box.

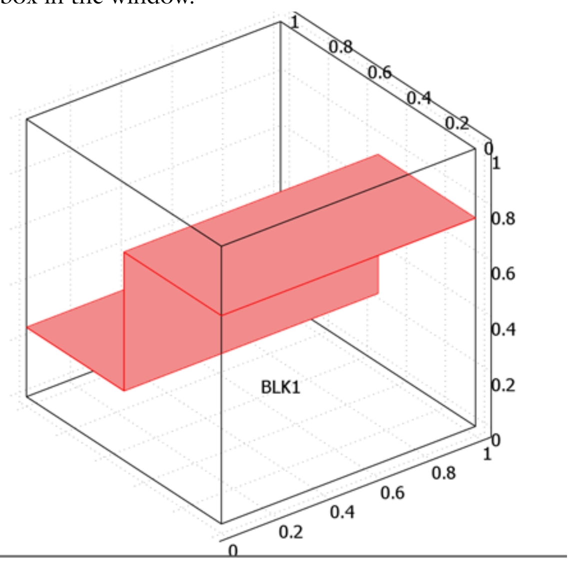
MODEL SETTINGS

Select the menu item **Physics>Model Settings**, then clear the **Simplify expressions** check box.

GEOMETRY

1 Go to the Draw toolbar and click the **Block** button. Click **OK** to accept the default dimensions, which create a unit block. Click the **Zoom Extents** button on the Main toolbar to center the block.

2 Now set up a 2D drawing plane to create the fracture. Select the menu item **Draw>Work-Plane Settings**. Click the **Face Parallel** tab. Expand the folder **BLK1** and highlight Face 2. Click **OK**. **Geometry 2** should appear with the outline of the box in the upper right corner. Click the **Zoom Extents** button on the Main toolbar to center the box in the window.



3 Changing the grid slightly makes it easier to draw the fracture. Select the menu item **Options>Axes/Grid Settings**. Click the **Grid** tab, then clear the **Auto** check box. In the **x-spacing** and **y-spacing** edit fields enter `0.25`. Click **OK**.

4 Next draw a 3-segment line to represent the fracture. Select the menu item **Draw>Specify Objects>Line**. In the **x-coordinates** edit field enter the sequence `0 0.5 0.5 1`, and in the **y-coordinates** edit field enter `0.75 0.75 0.25 0.25`. Click **OK**. This sets up segments with endpoints at (0, 0.75) (0.5, 0.75) (0.5, 0.25) (1, 0.25).

5 Now extrude the lines by 1 m to create a 3D object. With the lines still highlighted, select the menu item **Draw>Extrude**. In both the **Scale x** and **Scale y** edit fields enter `1`. Click **OK**.

OPTIONS

Define constants you need in building the model or during postprocessing.

1 Select the menu item **Options>Constants**, then enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
p0	1e5[Pa]	Initial pressure
thetas	0.3	Porosity matrix
Sfrac	4.4e-10[s^2*m/kg]	Fracture storage coefficient
kfrac	1e-7[1/m^2]	Fracture permeability
dfrac	0.1[mm]	Fracture thickness

2 Select the menu item **Options>Expressions>Scalar Expressions** and enter these names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
weak_frac	-kfrac/eta_esdl*dfrac*(pTx_test*pTx+pTy_test*pTy+pTz_test*pTz)	Fracture flow
dweak_frac	Sfrac*dfrac*p_time*p_test	Fracture storage

3 Select the menu item **Options>Expressions>Subdomain Expressions**, and from the **Subdomain selection** list choose **1** and **2**. Enter the following name and expression; when done, click **OK**.

NAME	EXPRESSION
matrix	1

4 Select the menu item **Options>Expressions>Boundary Expressions**. From the **Boundary selection** list select **6**, **8**, and **9**. Enter the following name and expression; when done, click **OK**.

NAME	EXPRESSION
frac	1

PHYSICS—MATRIX

Use the predefined equation options to set up the flow model for the matrix blocks.

1 Select the menu item **Physics>Subdomain Settings**. From the **Subdomain selection** list choose **1** and **2**. Enter the following settings; when done, click **OK**.

TERM	SELECTION	SUBDOMAINS 1, 2
Storage term	Specific Storage	
θ_s	Porosity	`thetas`
χ_f	Compressibility - fluid	`4.4e-10`
χ_p	Compressibility - solid	`1e-8`
κ_s	Permeability	`1e-11`
ρ_f	Density - fluid	`1000`
η	Dynamic viscosity - fluid	`0.001`

2 Select the menu item **Physics>Subdomain Settings**, then click the **Init** tab. In the **Initial value** edit field enter `p0`.

3 Select the menu item **Physics>Boundary Settings**. In the **Boundary condition** list verify that the setting is the default of **Zero flux/Symmetry**.

PHYSICS—FRACTURE

You must override the predefined boundary options to set up the flow model for the matrix blocks.

1 Select the menu item **Physics>Edge Settings**, then click the **Pressure** tab. In the **Edge selection** list choose **16** (the fracture inlet), then enter these settings:

QUANTITY	DESCRIPTION	VALUE/EXPRESSION
p_0	Pressure	`p0`
t_s	Starting time	`0`
t_f	Ending time	`1000`

For Edge 6 (the fracture outlet) enter these settings:

QUANTITY	DESCRIPTION	VALUE/EXPRESSION
p_0	Pressure	`p0-10[Pa/s]*t`
t_s	Starting time	`0`
t_f	Ending time	`1000`

2 Go to the menu item **Physics>Equation Systems>Boundary Settings**, then click the **Weak** tab. Highlight boundaries **6**, **8**, and **9**, then enter the following settings:

TERM	VALUE/EXPRESSION
weak	`weak_frac`
dweak	`dweak_frac`
constr	`0`

3 Click **Apply**, then click **Differentiate** to distribute the new information.

MESH GENERATION

1 Select the menu item **Mesh>Free Mesh Parameters**. On the **Global** page, in the **Predefined mesh sizes** list select **Coarse**.

2 Click the **Boundary** tab. Select Boundaries 6, 8, and 9, then in the **Maximum element size** edit field enter `0.075`.

3 Click the **Edge** tab. Select Edges 6 and 16, then in the **Maximum element size** edit field enter `0.025`. Click **OK**.

COMPUTING THE SOLUTION

1 Select the menu item **Solve>Solver Parameters**, then go to the **General** page.

2 Go to the **Time stepping** area, and in the **Times** edit field enter `0 1 10 50:50:1000`.

3 Go to the **Linear system solver** area, and in the like-named list choose **Conjugate gradients.** In the **Preconditioner** list select **Algebraic multigrid.** In the **Quality of multigrid hierarchy** edit field enter `9`. Click **Apply**, then click **OK**.

4 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

COMSOL Multiphysics allows you to create arbitrary variables and use them in postprocessing. The plots for this model use linear velocities that you first define. A short cut is to substitute the Darcy velocities `u_esdl`, `v_esdl`, `w_esdl`, and `U_esdl` or create the following variables and then update the model to recognize the new definitions.

1 Select the menu item **Options>Expressions>Scalar Expressions**. Add the following settings, each on its own row in the table; then click **OK**.

NAME	EXPRESSION
Ufrac_lin_avg	Ufrac_lin_sum/area_frac
Umatrix_lin_avg	Umatrix_lin_sum/volume_matrix

2 Select the menu item **Options>Expressions>Subdomain Expressions**. Select Subdomains 1 and 2, then enter the following settings, each on its own row in the table. When done, click **OK**.

NAME	EXPRESSION
umatrix_lin	u_esdl/thetas
vmatrix_lin	v_esdl/thetas
wmatrix_lin	w_esdl/thetas
Umatrix_lin	U_esdl/thetas

3 Select the menu item **Options>Expressions>Boundary Expressions**. Select Boundaries 6, 8, and 9, then enter the following settings, each on its own row in the table. When done, click **OK**.

NAME	EXPRESSION
ufrac_lin	-kfrac/eta_esdl*pTx
vfrac_lin	-kfrac/eta_esdl*pTy
wfrac_lin	-kfrac/eta_esdl*pTz
Ufrac_lin	sqrt(ufrac_lin^2+vfrac_lin^2+wfrac_lin^2)

4 Select the menu item **Options>Integration Coupling Variables>Subdomain Variables**. Select Subdomains 1 and 2, then enter the following settings, each on its own row in the table; when done, click **OK**.

NAME	EXPRESSION
Umatrix_lin_sum	Umatrix_lin
volume_matrix	1

5 Select the menu item **Options>Expressions>Boundary Expressions**. Select Boundaries 6, 8, and 9, then enter the following settings, each on its own row in the table; when done, click **OK**.

NAME	EXPRESSION
`Ufrac_lin_sum`	`U_esdl/dfrac`
`area_frac`	`1`

6 To calculate the expressions you have just defined, go to the **Solve** menu and select **Update Model**.

To generate Figure 2-29 on page 89:

1 Select the menu item **Postprocessing>Plot Parameters** and then click the **General** tab. In the **Plot type** area select the **Isosurface**, **Boundary**, **Arrow**, and **Max/min marker** check boxes.

2 Click the **Isosurface** tab. On both the **Isosurface Data** and **Color Data** pages, go to the **Predefined Quantities** list and select the flow solution **Pressure**. Select the **Vector with isolevels** option button, and in the associated edit field enter `91500:1500:100000`.

3 Click the **Boundary** tab. Go to the **Expression** edit field and enter `p*frac`. Because `frac` equals 1 on the fracture but zero everywhere else, multiplying `frac` by `p` gives the fluid pressure on the fracture instead of on all boundaries.

4 Go to the **Arrow** page. In the **Plot arrows on** list select **Boundaries**. In the **x-component edit field enter** `ufrac_lin*frac`; in the **y-component** edit field enter `vfrac_lin*frac`; and in the **z-component** edit field enter `wfrac_lin*frac`. In the **Arrow type** list select **Cone**.

5 Click the **Max/Min** tab and make sure you are on the **Subdomain Data** page. Clear the **Subdomain max/min data** check box. Click the **Boundary Data** tab, then select the **Boundary max/Min data** check box. In the Expression edit field enter `Ufrac_lin*frac`. Click **OK**.

6 Enhance the image with directed light. Select the menu item **Options>Visualization/Selection Settings**. Click the **Lighting** tab, and then select the **Headlight** check box. Click **OK**.

To generate Figure 2-30 on page 90:

1 Select the menu item **Postprocessing>Plot Parameters**, then click the **General** tab. In the **Plot type** area select the **Isosurface**, **Arrow**, **Slice**, **Boundary**, and **Max/min marker** check boxes. Switch among the desired output times from the figure by highlighting them in the **Solution at time** list.

2 Click the **Arrow** tab. In the **Plot arrows on** list select **Subdomains**. In the **x-component** edit field enter `umatrix_lin`, in the **y-component** edit field enter `vmatrix_lin`, and in the **z-component** edit field enter `wmatrix_lin`. Go to the **Arrow positioning** area. In the **Number of Points** column for all three options (**x**, **y**, and **z points**) enter `7`. In the **Arrow type** list select **Cone**.

3 Use a slice plot to see the linear velocity in the matrix block relative to the average value of the linear velocity on the fracture. Click the **Slice** tab and find the **Slice data** area. In the **Expression** edit field enter `Umatrix_lin/Ufrac_lin_avg`. Go to the **Slice positioning** area, and under the **Number of levels** column in both the **y-levels** and **z-levels edit fields** enter `0`. For **x-levels** select the option button in the **Vector with coordinates** column, and in the associated edit field enter `0.9`. In the **Fill style** list select **Wireframe**. Go to the Slice color area, and select the **Colormap** button, and in the associated drop-down list select **pink**.

4 Click **OK**.

To animate the solution sequence, select the menu item **Postprocessing>Plot Parameters** and then click the **Animate** tab. Change the image's **Width**, **Height** and **Frames per second** as appropriate. Click the **Start Animation** button.

To create the image that appears when opening the model file, add streamlines for viewing the matrix and fracture velocities simultaneously. To do so, continue with these instructions:

1 Select the menu item **Postprocessing>Plot Parameters** and go to the **General** page. In the **Plot type** area clear the **Slice** and **Max/min** marker check boxes. Select the **Streamline** check box.

2 Click the **Arrow** tab. In the **Plot arrows on** list select **Boundaries**. In the **x-component** edit field enter `ufrac_lin`, in the **y-component** edit field enter `vfrac_lin`, and in the **z-component** edit field enter `wfrac_lin`.

3 Go to the **Streamline** page. In the **x-component** edit field enter `umatrix_lin`, in the **y-component** edit field enter `vmatrix_lin`, and in the **z-component** edit field enter `wmatrix_lin`. Go to the **Start points** tabbed page. In the **Number of start points** edit field type `150`.

4 Click **OK**.

Variably Saturated Flow

This example uses the Richards' Equation application mode to assess how well geophysical irrigation sensors detect the true level of fluid saturation in variably saturated soils. Andrew Hinnell, Alex Furman, and Ty Ferre from the Dept. of Hydrology and Water Resources at the University of Arizona brought the example to us. They originally worked out the problem in COMSOL Multiphysics' PDE modes, but this discussion shares their elegant model reformulated in the Richards' Equation application mode.

A major challenge when characterizing fluid movement in variably saturated porous media lies primarily in the need to describe how the capacity to transmit and store fluids changes as fluids enter and fill the pore spaces. Experimental data for these properties are difficult to obtain. Moreover, the properties that change value as the soil saturates happen to be equation coefficients, which makes the mathematics notoriously nonlinear. The Richards' Equation application mode provides interfaces that automate the van Genuchten (Ref. 1) as well as the Brooks and Corey (Ref. 2) relationships for fluid retention and material properties that vary with the solution. This section discusses these interfaces and also explains how the application mode includes an interface that helps you use your own data or expressions to describe these properties (for details see "Interpolation for Unsaturated Flow" on page 115).

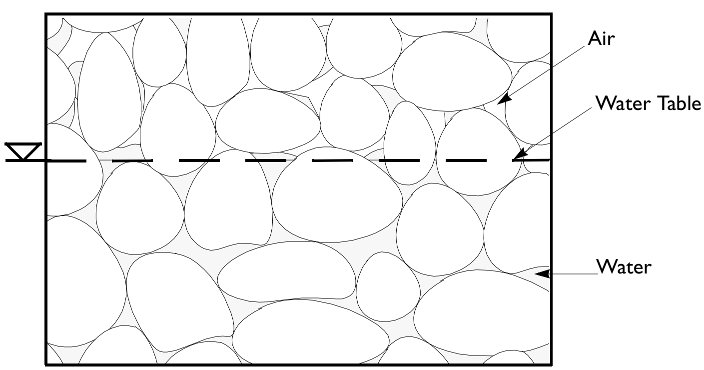


Figure 2-31: A variably saturated porous medium.

This example uses the model of Hinnell, Furman, and Ferre to characterize how the distribution of water changes around three impermeable sensors inserted into two different blocks of uniform soil partially saturated with water. The question for the model to address is this: Does the saturation localized around the sensor give a valid picture of the saturation within the total block?

This model demonstrates how to use the Richards' Equation application mode including the van Genuchten (Ref. 1) as well as the Brooks and Corey (Ref. 2) interfaces. The step-by-step instructions assist you in learning how to set up two separate equation systems in one COMSOL Multiphysics model file and then solve them simultaneously. It also explains a method to automate boundary and subdomain integrations using coupling variables—here the integrations estimate the average saturation around the sensors and within the soil blocks. For an example in which the soil retention and permeability properties are defined with experimental data, see the model "Interpolation for Unsaturated Flow" on page 115.

The following pages first contains an overview of the problem setup and review the equations and the boundary conditions. Following are a few details about implementing the integration-coupling variables and then a table of the data used in the model. The results of the simulations follow. Finally come detailed instructions for how to set up this model in the COMSOL Multiphysics user interface.

Model Definition

The problem setup is as follows. Two homogeneous columns of soil, each 2 m×2 m on a face, are partially saturated with water. A plot of the hydraulic properties of the first soil (Soil Type 1) fits the van Genuchten retention and permeability formulas. The other soil (Soil Type 2) has material properties that suit the Brooks and Corey formulas. Within each soil column are three impermeable rods, each with a 0.1 m radius. The rods are spaced at 0.5 m increments so they run horizontally down the center line of each block; see Figure 2-32. Just after the rods are emplaced, the pressure head is still uniform, but water begins to move vertically downward in steady drainage. Because all vertical slices down a block are identical, you can model a 2D cross section and observe the changes in the flow field for 900 s or 15 minutes.

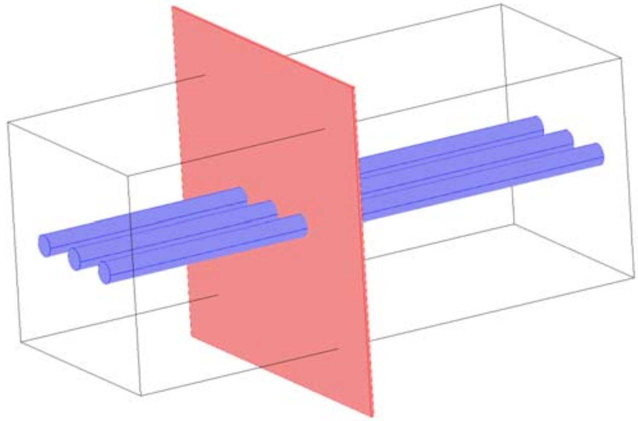


Figure 2-32: Soil block with three rods. Shaded plane represents a vertical cross section.

GOVERNING EQUATION

Richards' equation describes the unsaturated-saturated flow of water in the soils. In this problem you can use Richards' equation only for water because the air in the soil stays at atmospheric pressure because this model does not close the surface to the atmosphere or otherwise ramp up the air pressures. The governing equation for the model is

$$[C + \mathrm{Se}S]\frac{\partial H_p}{\partial t} + \nabla \cdot [-K\nabla(H_p + D)] = 0 \qquad (2\text{-}3)$$

Pressure head, H_p (m), is the dependent variable. C denotes specific moisture capacity (m^{-1}), Se is the effective saturation, S is a storage coefficient (m^{-1}), t is time, K is hydraulic conductivity ($\mathrm{m}^{-1}\cdot\mathrm{s}^{-1}$), and D is the coordinate (for example x, y, or z) for the vertical elevation. The equation does not show the volumetric fraction of water, θ, which is a constitutive relation that depends on H_p. Nonlinearities appear because C, Se, and K change with H_p and θ.

The first term in the equation explains that fluid storage can change with time during both unsaturated and saturated conditions. When the soil is unsaturated, the pores fill with (or drain) water. After the pore spaces completely fill, there is slight compression of the fluid and the pore space. The specific moisture capacity $C = \partial\theta/\partial H_p$ describes the change in fluid volume fraction θ with pressure head. The storage coefficient addresses storage changes due to compression and expansion of the pore spaces and the water when the soil is fully wet. To model the storage coefficient, this example uses the specific storage option, which sets $S = \rho_f g(\chi_p + \theta\chi_f)$. Here, ρ_f is the fluid density (kg/m^3), g is acceleration of gravity, while χ_p and χ_f are the compressibilities of the solid particles and fluid, respectively (kg/(m·s^2)).

The van Genuchten and the Brooks and Corey formulas that describe the change in C, Se, K, and θ with H_p require data for the saturated θ_s and θ_r liquid volume fractions and other dimensionless constants α, n, m, and l, which specify a particular media type. With the van Genuchten equations that follow, you consider the soil as being saturated when fluid pressure is atmospheric (that is, $H_p = 0$):

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

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

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

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

With the Brooks and Corey approach, an air-entry pressure distinguishes saturated ($H_p > -1/\alpha$) and unsaturated ($H_p < -1/\alpha$) soil as in

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

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

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

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

To find a unique solution to this problem, you must specify initial and boundary conditions. Initially, the column has uniform pressure head of H_{p0}. The boundary conditions are

$$\begin{array}{lll} \mathbf{n} \cdot [-\underline{K}\nabla(H_p + D)] & \partial\Omega & \text{Sides} \\ \mathbf{n} \cdot [-\underline{K}\nabla(H_p + D)] & \partial\Omega & \text{Rings} \\ H_p = H_{p0} & \partial\Omega & \text{Base} \\ H_p = H_{p0} & \partial\Omega & \text{Surface} \end{array}$$

where **n** is the normal to the boundary.

COMSOL Multiphysics Implementation—Integration Coupling Variables

Integration coupling variables in COMSOL Multiphysics calculate integrals for arbitrary expressions on a given type of model domain (the source) and make that information available elsewhere in the model (the destination). As such, you can classify coupling variables by the source of the information. For example, boundaries, subdomains, and points are different types of sources that arise within every 2D model.

To calculate the average value of the effective saturation, Se, at the rod and throughout the soil requires two types of integration coupling variables: boundary coupling variables for the rod-soil boundary, and subdomain coupling variables for the soil. If the average saturation is

$$\overline{\mathrm{Se}} = \frac{\int \mathrm{Se}\, d\sigma}{\int d\sigma},$$

σ denotes the domain. The expression consists of two integrals. The numerator sums the effective saturation values along the boundary or within the subdomain. The denominator sums the boundary length or subdomain area (2D).

This model makes modest use of coupling variables to calculate saturations and compares them during postprocessing. In that coupling variables are so clever, it is worth mentioning a use or two. You can use them to evaluate, for example, a flux on an outlet and return the information as a source term on the inlet to link physics on separately meshed geometries within one model. And this is just the beginning. For more information on this topic, refer to “Using Coupling Variables” on page 255 in the *COMSOL Multiphysics User’s Guide*.

DATA

The following table gives the data needed to complete the two example problems:

VARIABLE	UNITS	DESCRIPTION	VAN GENUCHTEN	BROOKS & COREY
g	m/s^2	Gravity	9.82	9.82
ρ_f	kg/m^3	Fluid density	1000	1000
χ_p	$m\ s^2\ kg^{-1}$	Compressibility of solid particles	1e-8	1e-8
χ_f	$m\ s^2\ kg^{-1}$	Compressibility of fluid	$4.4\cdot 10^{-10}$	$4.4\cdot 10^{-10}$
K_s	$m\ s^{-1}$	Saturated hydraulic conductivity	$8.25\cdot 10^{-5}$	$5.83\cdot 10^{-5}$
θ_s		Porosity/void fraction	0.43	0.417
θ_r		Residual saturation	0.045	0.02
α	m^{-1}	alpha parameter	14.5	13.8
n		n parameter	2.68	0.592
m		m parameter	1-1/n	n/a
l		Pore connectivity parameter	0.5	1
H_{p0}	m	Specified pressure	-0.06	-0.2
H_{p0}	m	Initial pressure	-0.06	-0.2

Results

Figure 2-33 and Figure 2-34 are solutions to the Richards' equation problem of Prof. Ty Ferre, Andrew Hinnell, and Alex Furman from the University of Arizona's Department of Hydrology and Water Resources. Each figure gives results for similar variably saturated flow problem posed for different soil types. Each snapshot shows effective fluid saturation (surface plot), pressure head (contours), and fluid velocities (arrows). The flow field varies around the rods but remains largely uniform over the remainder of each block.

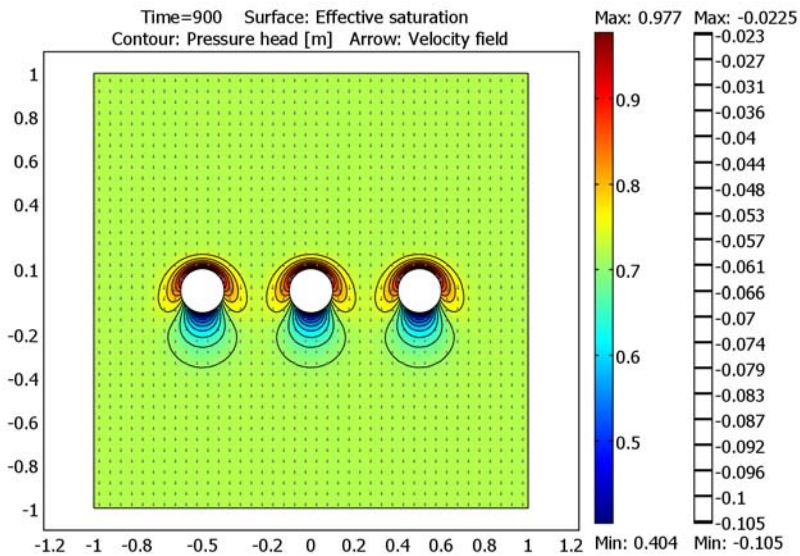


Figure 2-33: Solution for effective saturation (surface plot), pressure head (contours), and velocity (arrows) at 30 minutes for Soil Type 1 (van Genuchten).

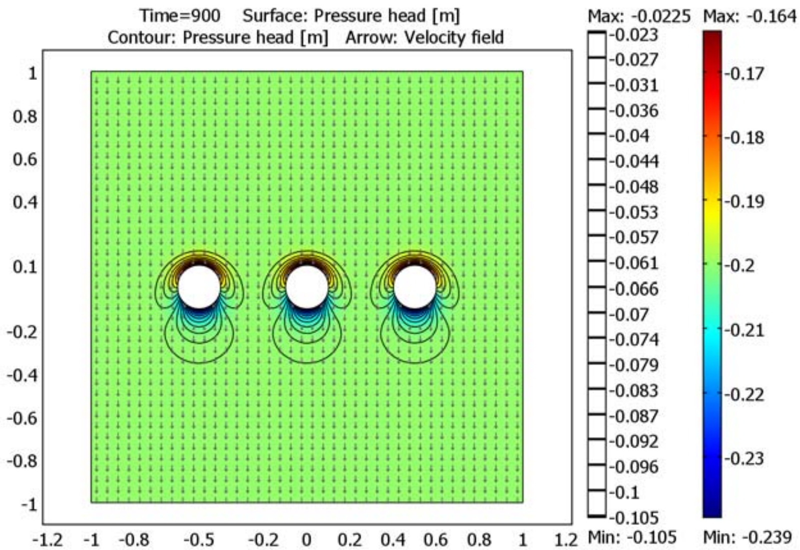


Figure 2-34: Solution for effective saturation (surface plot), pressure head (contours), and velocity (arrows) at 30 minutes for Soil Type 2 (Brooks and Corey).

Figure 2-35 shows the effective saturation evolving over time at the rod-soil boundary. In the figure, the solid lines denote the solution for Soil Type 1, and the dashed lines

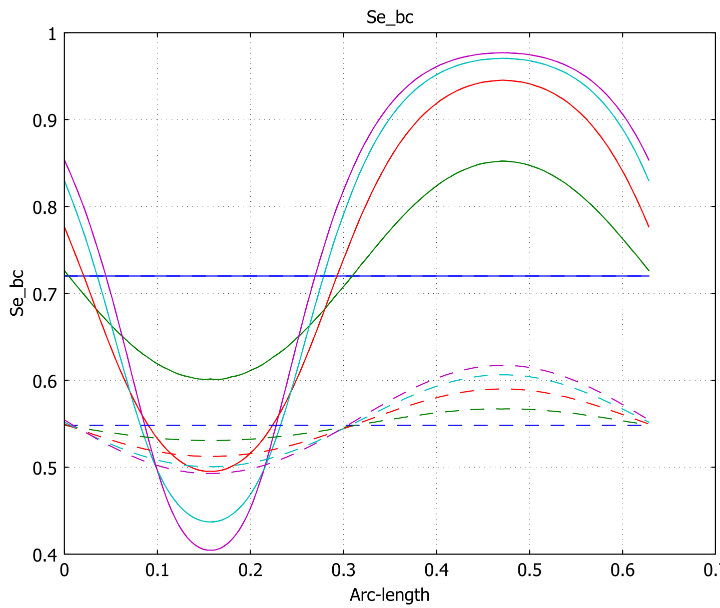


Figure 2-35: Effective saturation around the center rod in Soil Type 1 (solid lines) and Soil Type 2 (dashed lines). Results are for 0 s, 60 s, 300 s, 600 s, and 900 s.

correspond to Soil Type 2. Because the boundary is a circle, the x-axis in the figure is an arc length, and those < 0.5 refer to the semicircle below the rods. In the results, the initial value of effective saturation plots as a horizontal line. The soil is wetter just above the rods than below them. That the saturation around Soil Type 1 extends beyond the arc length distance of 0.5 suggests that the entire boundary will get completely wet with time.

Figure 2-36 compares the average fluid saturations at the rod boundary with the average within the two blocks of soil. The range of effective saturation estimates at the rod boundary appears as a scatter plot for different time steps. The solid line is the integral of the effective saturation at the rod boundary. The dashed line is the integral of effective saturation for the block. Clearly the average effective saturation at the rods increases with time, but the average for the block does not change. While the effects shown here are more pronounced in Soil Type 1 than Soil Type 2, the results call to question whether the sensors can accurately assess soil moisture if kept in situ for long times.

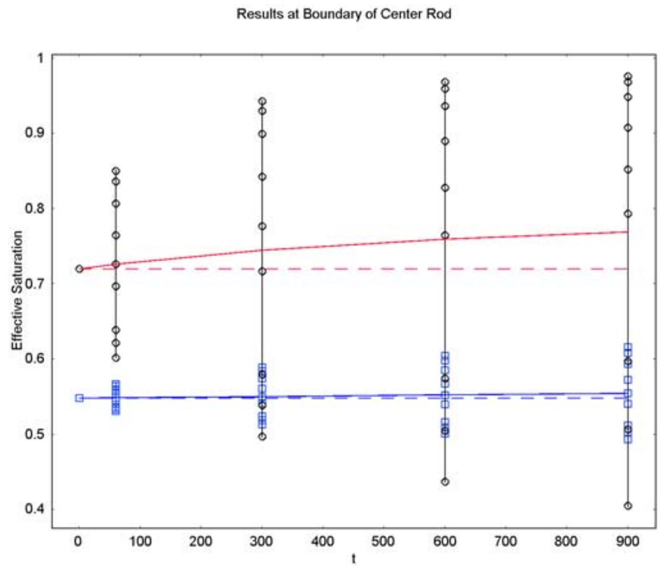


Figure 2-36: Average effective saturation at sensor circumference (solid lines) and overall soil block (dashed lines) for Soil Type 1 (top set) and Soil Type 2 (bottom set). Also shown is the range of effective saturation at the rod circumference for Soil Type 1 (circles) and Soil Type 2 (squares).

References

1. M.Th. van Genuchten, "A closed-form equation for predicting the hydraulic of conductivity of unsaturated soils," *Soil Sci. Soc. Am. J.*, vol. 44, pp. 892–898, 1980.

2. R.H. Brooks and A.T. Corey, "Properties of porous media affecting fluid flow," *J. Irrig. Drainage Div., ASCE Proc*, vol. 72 (IR2), pp. 61–88, 1966.

Model Library path: `Earth_Science_Module/Fluid_Flow/varsat`

Modeling Using the Graphical User Interface

To begin the model, first set up a geometry with an *x-z* axis, then add two Richards' Equation application modes.

MODEL NAVIGATOR

1 Open the **Model Navigator**, and in the **Space dimension** list select **2D**.
2 Click the **Multiphysics** button.
3 Click the **Add Geometry** button. In the **Independent variables** edit field change the entry to read `x z y` in that order. Click **OK**.
4 In the list of application modes select **Earth Science Module>Fluid Flow>Richards' Equation>Pressure head analysis>Transient analysis**. In the **Application mode name** edit field replace the current data with `bc` (for the Brooks & Corey method). Click the **Add** button and leave the dialog box open.
5 With the application mode **Earth Science Module>Fluid Flow>Richards' equation>Pressure head analysis>Transient analysis** still selected, go to the **Application mode name** edit field and enter `vg` (for the van Genuchten analysis). Click **Add**, then click **OK**.

APPLICATION SCALAR VARIABLES

To set the vertical direction in the model, go to the **Physics** menu and select **Scalar Variables.** Make the following modifications to the defaults, and then click **OK**.

NAME	EXPRESSION
D_vg	z
D_bc	z

GEOMETRY MODELING

Create the geometry by drawing a rectangle and subtracting three circles from it.

1 Go to the Draw toolbar on the left side of the user interface and choose the **Centered Rectangle/Square** button. Draw a square centered on the origin, with an upper left corner at $x = -1, z = 1$ and a lower right corner at $x = 1, z = -1$.
2 Go to the **Draw** menu and select **Specify Objects>Circle**. In the resulting dialog box enter these settings; when done, click **OK**.

NAME	EXPRESSION
radius	`0.1`
x	`-0.5`
z	`0`

3 Select the menu item **Draw>Modify>Array**. In the **Displacement x** edit field enter `0.5`, and in the **Array size x** edit field enter `3`. Click **OK**.

4 Select all the objects (press Ctrl+A). Click the **Difference** button on the Draw toolbar.

5 Click the **Zoom Extents** button on the Main toolbar to center the geometry in the field of view.

OPTIONS AND SETTINGS

Now set up variables to integrate the effective saturation in the subdomain and along the rod boundary.

1 Select the menu item **Options>Integration Coupling Variables>Subdomain Variables**. Enter data from the following table to create the needed variables; when done, click **OK**.

NAME	EXPRESSION
sint_vg	Se_vg
sint_bc	Se_bc
sarea	1

2 Select the menu item **Options>Integration Coupling Variables>Boundary Variables**. Select boundaries 9 through 12. Enter data from this table to create the needed variables; when done, click **OK**.

NAME	EXPRESSION
bint_vg	Se_vg
bint_bc	Se_bc
blength	1

PHYSICS SETTINGS

Subdomain Settings—Soil Type 1 (van Genuchten)

First set up the model for Soil Type 1, which you build with the van Genuchten retention and permeability relationships.

1 Select the menu item **Physics>Subdomain settings**. On the **Coefficients** page enter the following settings:

TERM	VAN GENUCHTEN
Constitutive relation	van Genuchten
θ_s	0.43
θ_r	0.045
Storage term	Specific storage

TERM	VAN GENUCHTEN
χ_f	4.4e-10
χ_p	1e-8
K_S	8.25e-5
ρ_f	1000

2 Click the **van Genuchten** tab and enter these settings:

TERM	VAN GENUCHTEN
α	14.5
n	2.68
l	0.5

3 Click the **Init** tab. In the **Initial value** edit field for $\mathbf{H_{pt(0)}}$ enter `-0.06`.

4 Click **OK**.

Boundary conditions

From the **Physics** menu select **Boundary Settings.** Set these boundary conditions; when done, click **OK**.

BOUNDARY	BOUNDARY CONDITION	VARIABLE	VALUE
2, 3	Pressure head	H_{p0}	-0.06
1, 4–16	Zero flux/Symmetry		

Subdomain Settings—Soil Type 2 (Brooks and Corey)

Create a second application in the same model file for Soil Type 2 using the Brooks and Corey parameterization approach.

1 From the **Multiphysics** menu select **Richards' Equation (bc)**.

2 From the **Physics** menu select **Subdomain Settings**, then click the **Coefficients** tab. Enter the following expressions.

SYMBOL	BROOKS & COREY
Constitutive relation	Brooks & Corey
θ_s	0.417
θ_r	0.02
Storage term	Specific storage
χ_f	4.4e-10
χ_p	1e-8

SYMBOL	BROOKS & COREY
K_S	`5.8333e-5`
ρ_f	`1000`

3 Click the **Brooks & Corey** tab, then enter these settings:

SYMBOL	BROOKS & COREY
α	`13.8`
n	`0.592`
l	`1`

4 Click the **Init** tab. In the **Initial value** edit field for $\mathbf{H_{pt(0)}}$ enter `-0.2`.

5 Click **OK**.

Boundary conditions

From the **Physics** menu select **Boundary Settings.** Set these boundary conditions; when done, click **OK**.

BOUNDARY	BOUNDARY CONDITION	VARIABLE	BROOKS & COREY
2, 3	Pressure head	H_{p0}	`-0.2`
1, 4–16	Zero flux/Symmetry		

MESH GENERATION

1 Select the menu item **Mesh>Free Mesh Parameters**.

2 Click the **Boundary** tab. Select the three circles in the model domain; to do so, left-click the mouse in the user interface and draw a box around the circles. Then in the **Maximum element size** edit field enter `0.025`. Click **OK**.

COMPUTING THE SOLUTION

1 Select the menu item **Solve>Solver Parameters**. Find the **Solver** list, and verify that **Time dependent** is selected.

2 Remaining on the **General** page, go to the **Time stepping** area. To specify output times for the model, go to the **Times** edit field and enter `0 60 300 600 900`. Click **OK**.

3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 2-33 on page 105, follow these steps:

1 Select the menu item **Postprocessing>Plot Parameters**.
2 Go to the **General** page. In the **Plot type** area select the **Surface**, **Contour**, and **Arrow** check boxes.
3 Click the **Surface** tab. In the **Surface data** area go to the **Expression** edit field and enter `Se_vg`, typing over the current expression. `Se_vg` stands for effective saturation (the `Se`) calculated with the application mode named vg (`_vg`).
4 Click the **Contour** tab. In the **Contour data** area go to the **Predefined quantities** list and select **Richards' Equation (vg)>Pressure head**. In the **Contour color** area select **Uniform color** option button. Click the **Color** button, select black, then click **OK**.
5 Click the **Arrow** tab. In the **Arrow data** area go to the **Predefined quantities** list and select **Richards' Equation (vg)>Velocity field**. Go to the **Arrow positioning area**. In the **Number of points** edit fields for both **x points** and **z points** enter `40`. Click the **Color** button, then choose gray; click **OK**.
6 Return to the **General** page. Click the **Title** button, enter a title as appropriate, and then click **OK**.
7 Click **OK** to close the **Plot Parameters** dialog box.

To create Figure 2-34 on page 106 for the **Richards' equation (bc)** application mode, repeat the steps for Figure 2-33—except this time on the **Surface** page in the **Expression** edit field you enter `Se_bc`.

To generate Figure on page 107, continue with these steps:

1 Select the menu item **Postprocessing>Domain Plot Parameters**.
2 Click the **Line/Extrusion** tab. Go to the **y-axis data** area, and in the **Expression** edit field enter `Se_vg`. In the **Boundary Selection** list select **9** through **12**. Click **Apply**.
3 To add the second set of results, click the **General** tab and also select the **Keep current plot** check box. Then repeat the steps just outlined for Soil Type 2 (Brooks and Corey)—except this time return to the **Line/Extrusion** page and in the **Expression** edit field enter `Se_bc`.
4 Go back to the **General** page. Clear the **Keep current plot** check box, then click **OK**.

To generate Figure 2-36 on page 108, continue with these steps:

1 Select the menu item **Postprocessing>Domain Plot Parameters**. Go to the **General** page, then select the **Keep current plot** check box. Click **Apply**.
2 Now you want to add the distribution of effective saturation estimates at each output time. On the **Line/Extrusion** page, go to the **y-axis data** area and in the **Expression** edit field enter `Se_vg`. In the **Boundary selection** list select **9** through **12**.

3 Go to the **x-axis data** area and select **Expression** option button. In the **Expression** edit field enter `t`, then click **OK**.

4 Click the **Line settings** button at the bottom of the dialog box. Modify the line and symbol settings as desired. Click **OK**.

5 The next step is to overlay lines for the average saturation on the boundary. Click the **Point** tab, and in the **Point selection** list select an arbitrary point in the model domain. In the **Expression** edit field enter `bint_vg/blength`. Click the **Line Settings** button, modify these settings as desired, then click **OK**. Click **Apply**.

6 Now plot the average saturation over the subdomain. Go to the **Point** page, and in the **Point selection** list select an arbitrary point in the model domain. In the **Expression** edit field enter `sint_vg/sarea`. Click the **Line Settings** button, modify these settings as desired, then click **OK**. Click **Apply**.

7 To overlay results obtained with Soil Type 2 repeat Steps 2 through 6 using the corresponding expressions for application mode 2. Alternatively, to generate a separate plot for application mode 2, click the **General** tab and the **Plot in** list and choose **New figure**. Then repeat Steps 2 through 6 for application mode 2.

Interpolation for Unsaturated Flow

Variably saturated flow models are notoriously difficult to parameterize because several material and hydraulic properties change values as the pressure and saturation levels fluctuate. Ideally, experimentalists prefer to use their hard-earned data in a model rather than finding best-fit analytical expressions. This example demonstrates how to incorporate experimental data directly into a simulation. Nathan Miller of Michigan State University pioneered this approach in his COMSOL Multiphysics model of fluid, heat, and gas movement to a turtle nest.

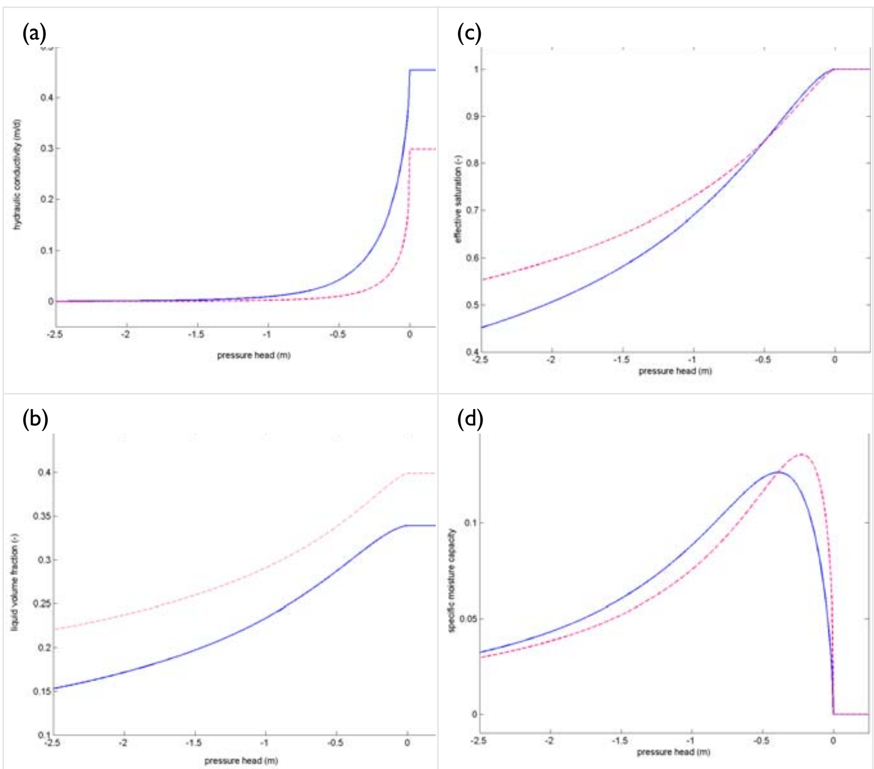


Figure 2-37: Analytical (lines) and interpolated (markers) estimates of properties that depend on Hp. Shown for the upper soil layer (dashed line) and lower soil layer (solid line) are: hydraulic conductivity, K (a); liquid volume fraction, θ *(b); effective saturation, Se, (c); and specific moisture capacity, C (d).*

This example uses interpolation between experimental data points to estimate values of the equation coefficients Se, θ, K, and C (see Equation 2-3 on page 101) that fit the solution for the pressure-head, H_p, during a flow simulation.

The interpolation model described here builds on the flow model described in "Variably Saturated Flow" on page 99. In variably saturated transport, you define the equation coefficients Se, θ, K, and C, which vary with pressure head, H_p, using analytic expressions from van Genuchten (Ref. 1) and that are available in the Richards' Equation application mode. For this interpolation model, the author parameterized the same basic flow problem by sampling from analytic calculations to obtain a fictitious experimental dataset and interpolating between the scattered points. At the close of the model, this discussion compares results from interpolated material properties to those obtained with analytical calculations.

Model Definition

Example 4 from the SWMS2D manual (Ref. 2) inspired the basic flow problem set out in this model. In that example, a ring of 0.25 m radius sits at the ground surface. Within it water ponds to a depth of 0.01 m. The ring is bottomless, so water moves from the ring into the soil. The problem examines the flow into a 1.3 m long soil column of radius 1.25 m.

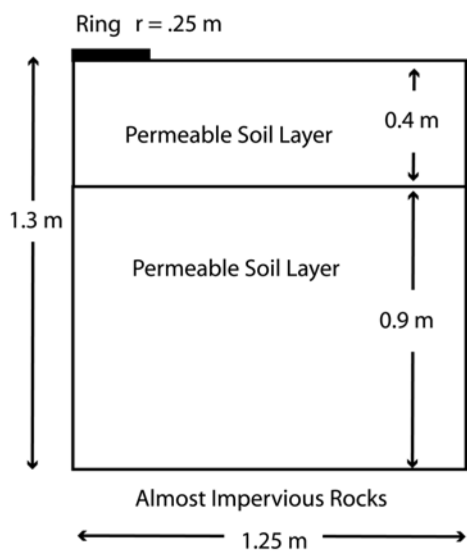


Figure 2-38: Geometry showing infiltration ring on top of a soil column.

The soil is layered; the upper soil layer is 0.4 m thick, and the lower layer sits on top of relatively impermeable soil. At the ground surface beyond the ring, there is no entry. The only flow exit is a small amount of leakage from the base. The center line of the ring is an axis of symmetry. The distribution of pressure head is known at an initial time. For more information about this flow model, see the example "Variably Saturated Flow" on page 99.

FLUID FLOW

Richards' equation governs fluid flow in variably saturated porous media. A benefit of the form of Richards' equation used here is that it allows for changes in storage related to increasing and decreasing moisture as well as storage changes due to compression and expansion when the soil is fully wet. The equation is

$$[C + \mathrm{Se}\, S]\frac{\partial H_p}{\partial t} + \nabla \cdot [-K_s k_r \nabla (H_p + D)] = Q_s$$

where C is specific moisture capacity (m^{-1}); Se is the effective saturation; S denotes the storage coefficient (m^{-1}); H_p equals the pressure head (m); t is the time (d); K_s represents the hydraulic conductivity ($\mathrm{m}^{-1} \cdot \mathrm{d}^{-1}$); k_r gives the relative permeability; D is the coordinate (for example x, y, or z) for the vertical elevation; and Q_s represents the fluid source defined by volumetric flow rate per unit volume of soil (d^{-1}). Here S equals the difference between the liquid volume fraction at saturation, θ_s, and the residual liquid volume fraction, θ_r, or specific yield per unit length.

Changes in pressure head and elevation head drive fluid through the soil. K, θ, C, and Se vary under unsaturated conditions (for example, $H_p < 0$), and they reach a constant value when the system saturates (for example, $H_p \geq 0$). In a typical experimental station, you conduct simultaneous tests to identify how the hydraulic conductivity function $K = K_s\, k_r$ ($\mathrm{m}^{-1} \cdot \mathrm{d}^{-1}$) and the volume fraction of fluid in the soil, θ, change with H_p. The specific moisture capacity, C, relates changes observed in the soil moisture, θ, to the change in pressure head, H_p. The relative permeability, k_r explains how the transmissive properties of the soil, K, vary with pressure head, H_p. The effective saturation, Se, denotes the value of θ scaled to a maximum of 1.

This example employs interpolation functions with a fictional set of experimental data consisting of K and θ data for different values of H_p. It uses interpolation when the soil is unsaturated ($H_p < 0$) to estimate K and θ for different values of the solution, H_p. The model defines C by the "slope" in the θ versus H_p values. Se is a scaled version of the θ results. The parameterization is as follows:

$$\theta = \begin{cases} f(H_p) & H_p < 0 \\ \theta_s & H_p \ge 0 \end{cases}$$

$$\mathrm{Se} = \begin{cases} (\theta - \theta_r)/(\theta_s - \theta_r) & H_p < 0 \\ 1 & H_p \ge 0 \end{cases}$$

$$C = \begin{cases} \partial\theta/\partial H_p & H_p < 0 \\ 0 & H_p \ge 0 \end{cases}$$

$$k_r = \frac{K}{K_s}\begin{cases} f(H_p) & H_p < 0 \\ 1 & H_p \ge 0 \end{cases}$$

where pressure head at saturation is atmospheric (that is, $H_p = 0$). Here, θ_s and K_s denote the soil's total porosity and the saturated hydraulic conductivity.

For the boundary conditions, the pressure head in the ring is constant, and no flow exits in the surface outside the pressure ring. The sides are impermeable. The vertical boundary on the inside of the ring is a line of symmetry, and the model approximates the small amount of leakage from the base, N_0, as being $0.01K_s$. In summary, the boundary conditions are:

$$\begin{array}{ll} H_p = H_{p0} & \partial\Omega \ \text{Ring} \\ \mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = 0 & \partial\Omega \ \text{Surface} \\ \mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = 0 & \partial\Omega \ \text{Sides} \\ \mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = 0 & \partial\Omega \ \text{Symmetry} \\ \mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = N_0 & \partial\Omega \ \text{Base} \end{array}$$

where **n** is the outward unit normal to the boundary. Initially, the column has a specified distribution of pressure head of H_{p0}. Here, you define the initial pressures with an equation that approximates the distribution shown for June 1982 in Example 4 from SWMS2D (Ref. 2).

Implementation: Interpolation from Scattered Data

The "experimental data" are 25 data points sampled at regular H_p intervals from K and θ values calculated with the following formulas (Ref. 1). The data also include repeats of the constants for extreme pressure heads to prevent extrapolating beyond the range of physical property values. You can calculate the sampled distributions from

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

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

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

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

where α, n, m, and l are dimensionless constants that specify a particular media type, and $m = 1 - 1/n$.

Implementation: Interpolation from Experimental Data

This analysis finds the correct value of $K = K_s k_r$ and θ for the solution H_p using COMSOL Multiphysics commands to interpolate between experimental data points. You calculate Se based on the interpolated θ estimates, then use COMSOL Multiphysics' automated differentiation commands (for example, `diff` and `pdiff`) to define C as the derivative of θ with respect to H_p.

Interpolation in COMSOL Multiphysics is straightforward. You open a dialog box from the **Options** menu, import data from a text file, assign a name to the interpolation function, and use that name where the function is needed, here the **Subdomain Settings** dialog boxes.

The step-by-step instructions that follow create interpolation functions for each K and θ in two layers, giving a total of four functions. The example laid out here uses precreated files that contain the pressure head with corresponding property values. For the hydraulic conductivity function, $K = K_s k_r$, in Subdomain 1, the name of the data file is `K_sub1.txt`. Within that file, the pressure-head data make up the first string of numbers, and the corresponding hydraulic-conductivity values follow. For example, the final five entries from `K_sub1.txt` read

```
%grid
-0.3 -0.2 -0.1 0.0 100
%data
 0.0903 0.1376 0.2199 0.4540 0.454
```

In this sample from the data file, `grid` denotes that H_p data follow, and `data` denotes that corresponding K data come next.

Note: The file gives only unsaturated properties, but you repeat the saturated hydraulic conductivity, K_s, of 0.454 m/d for a positive pressure head of 100 m to prevent interpolation beyond the range of the data.

To activate the new functions you just created, simply enter the function name (for example, `K_sub1`) along with the argument (for example, the pressure head `Hp`). For the relative permeability, k_r, the command is:

```
kr = K_sub1(Hp)/Ks
```

Find out more about interpolation commands by referring to the *COMSOL Multiphysics User's Guide*. You can use the interpolation commands with spatial data as well. For a model that employs these interpolation commands to map out spatially varying material properties, see "A Rock Fracture Flow Model" on page 270 in the *COMSOL Multiphysics Model Library.*

DATA

The following table provides the constants and the expressions used in this model. The data come from the example in Ref. 2. The expressions for implementing the interpolation commands appear in the user-interface instructions.

VARIABLE	UNIT	DESCRIPTION	UPPER LAYER	LOWER LAYER
K_s	m/d	Saturated hydraulic conductivity	0.298	0.454
q_s		Porosity/void fraction	0.399	0.339
q_r		Residual saturation	0.0001	0.0001
H_{ps}	m	Pressure head in ring	0.01	
H_{p0}	m	Initial pressure head	-(z+1.2)*(z<-.4)+(-(z+1.2)-.2*(z+.4))*(-.4<=z)	-(z+1.2)*(z<-.4)+(-(z+1.2)-.2*(z+.4))*(-.4<=z)

The next table summarizes the parameters used in calculating the van Genuchten distributions for Se, K, and θ.

VARIABLE	UNITS	DESCRIPTION	UPPER LAYER	LOWER LAYER
K_s	m/d	Saturated hydraulic conductivity	0.298	0.454
q_s		Porosity/void fraction	0.399	0.339
q_r		Residual saturation	0.0001	0.0001
α	m^{-1}	alpha parameter	1.74	1.39
n		n parameter	1.3757	1.6024
m		m parameter	1-1/n	
l		Pore connectivity parameter	0.5	0.5

Results

Figure 2-37 on page 115 shows the values for K, θ, Se, and C estimated here by interpolation from "experimental" datasets consisting of 25 points sampled from analytic distributions (Ref. 1). The sets of interpolated and analytic estimates for the upper and the lower soil layers match closely.

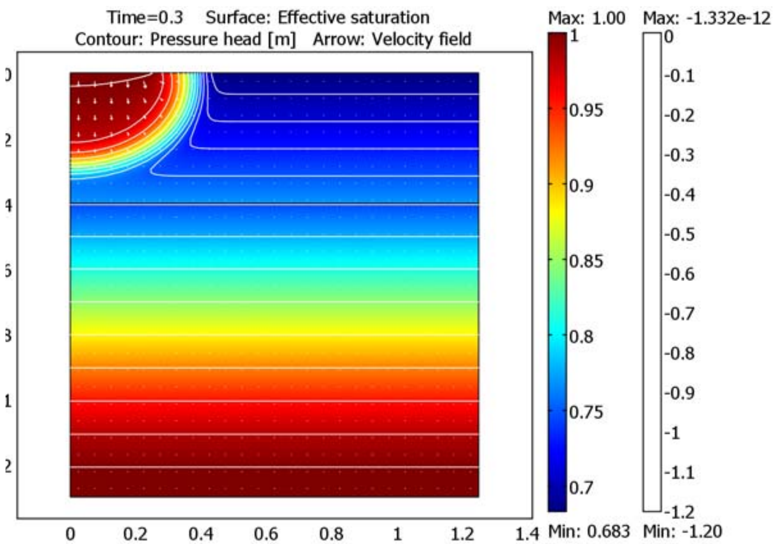


Figure 2-39: Solution for variably saturated flow simulated with properties interpolated from experimental data. Results shown are effective saturation (surface plot), pressure head (contours), and velocity (arrows) at 0.3 days.

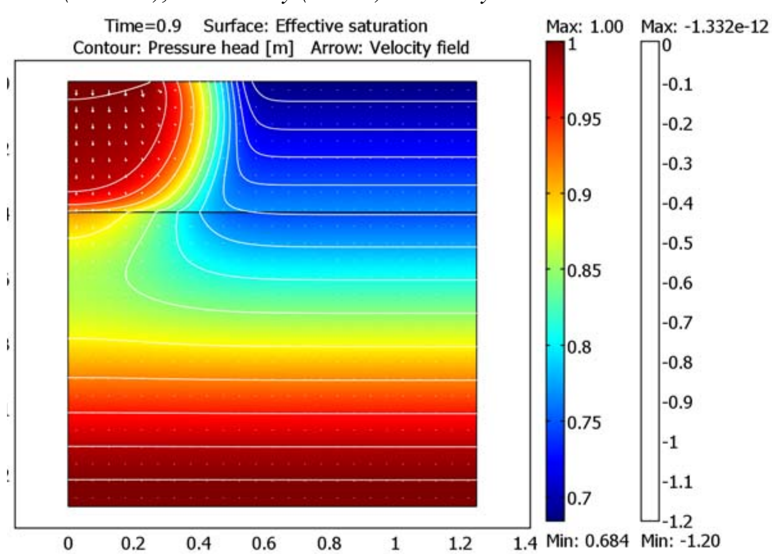


Figure 2-40: Solution for variably saturated flow simulated with material properties interpolated from experimental data. Results shown are effective saturation (surface plot), pressure head (contours), and velocity (arrows) at 1 day.

The two nearby figures show the solutions of variably saturated flow modeled with interpolated K, θ, Se, and C values at 0.25 days and 1 day. They show effective saturation (surface plot), pressure head (contours), and velocities (arrows). At day 0.25, the fluid moves primarily below the ponded region.

By the end of one day, the water moves deeper within the volume. Because very little fluid exits from the base, the soil gradually saturates upward with time. The results are so similar to values obtained with closed-form equations to define K, θ, Se, and C that this discussion does not repeat them; the curious reader should refer to "Variably Saturated Flow" on page 99.

Figure 2-41 is a plot of pressure heads simulated in COMSOL Multiphysics with linear and nearest neighbor interpolation to define K, θ, Se, and C from experimental data. It shows results for various depths along the line x = 0.2, and it also illustrates similar values for simulations with closed-form analytic estimates of K, θ, Se, and C. Which interpolation method is appropriate for a model depends on the property values and the number of data, among other things.

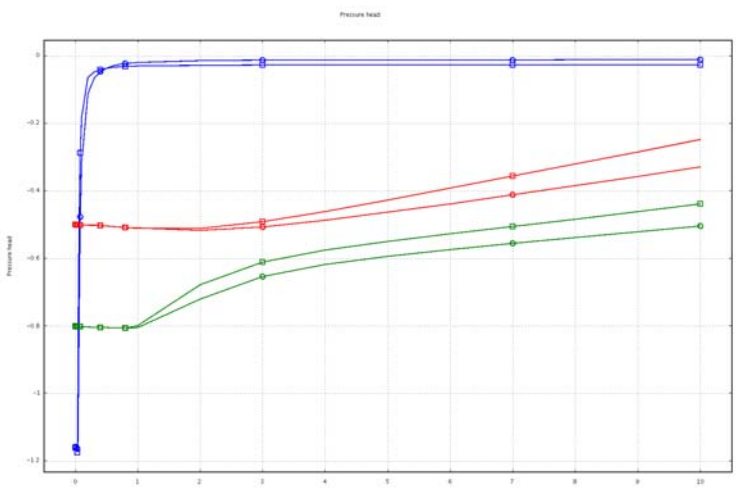


Figure 2-41: Pressure heads simulated with linear interpolation (squares) and analytic formulas (circles) for retention and permeability functions. Results are for x y coordinates, in m, (0.2, -0.1), (0.6, -0.4), and (1.0, -0.7).

This example demonstrates how to simulate variably saturated flow using fluid-retention and permeability values obtained by interpolation from experimental data, which you here import into COMSOL Multiphysics as a text file. Then use the COMSOL Multiphysics interpolation functions and the Richards' equation user-definition options to parameterize the model. The user-definition options also allow you to enter arbitrary expressions for these properties, for example, to define how permeability and moisture content vary during unsaturated conditions, and COMSOL Multiphysics can automate finding the solution.

References

1. M.Th. van Genuchten, "A closed-form equation for predicting the hydraulic of conductivity of unsaturated soils," *Soil Sci. Soc. Am. J.*, vol. 44, pp. 892–898, 1980.

2. J. Simunek, T. Vogel, and M.Th. van Genuchten, *The SWMS_2D code for simulating water flow and solute transport in two-dimensional variably saturated media, Version 1.1*, Research Report No. 132, U.S. Salinity Laboratory, USDA, Riverside, CA, 1994.

Model Library path: `Earth_Science_Module/Fluid_Flow/interpolation`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Open the Model Navigator, and from the **Space dimension** list select **Axial symmetry (2D)**.
2. From the list of application modes select **Earth Science Module>Fluid Flow>Richards' Equation>Pressure head analysis>Transient analysis**, then click **OK**.

GEOMETRY MODELING

Create the geometry by drawing one rectangle and adding two lines.

1. From the **Draw** menu select **Specify Objects>Rectangle**. Enter the following settings, then click **OK**.

PARAMETER	EXPRESSION
width	`1.25`
height	`1.3`

PARAMETER	EXPRESSION
r	0
z	-1.3

2 Go to the Main toolbar and click the **Zoom Extents** button.

3 Return to the **Draw** menu and select **Specify Objects>Rectangle**. Specify the following shape, then click **OK**.

PARAMETER	EXPRESSION
width	1.25
height	0.4
r	0
z	-0.4

4 Return to the **Draw** menu and select **Specify Objects>Line**. In the **r coordinate** edit field enter `0 0.25`, and in the **z coordinate** edit field enter `0 0`. Click **OK**.

OPTIONS AND SETTINGS

Now set up the interpolation routines. You interpolate for six datasets. Import the data as files and assign a name that you use elsewhere to call for the interpolated values. In the data files, the H_p values are the "grid," and the corresponding parameter values are the "data." The datafiles are available once the Earth Science Module has been installed.

1 Choose **Options>Functions**. In the **Defined Functions** area, click the **New** button.

2 To define the hydraulic conductivity in Subdomain 1 (the lower layer), go to the **Function name** edit field and enter `K_sub1`. Select **Interpolation** and choose **File** from the **Use data from** list. Click **Browse**. Then find the file `K_sub1.txt`, in `Models/Earth_Science_Module/Fluid_Flow` in the COMSOL installation directory. Click **OK**.

3 Repeat this process for the files `th_sub1.txt`, `K_sub2.txt`, and `th_sub2.txt`. Be sure to click **New** before starting to create each new function. After you have named and imported data for each function, click **Apply**.

4 Click **OK** to close the **Functions** dialog box.

PHYSICS SETTINGS

Application Scalar Variables

To set the vertical direction and gravitational constant in the model, go to the **Physics** menu and select **Scalar Variables**. Make the following modifications to the defaults. Here you convert from seconds to days by multiplying by the number of seconds per day, and square the quantity because you are dealing with acceleration. Click **OK**.

NAME	EXPRESSION
D_esvr	z
g_esvr	9.82*86400*86400

Subdomain Settings

Set up the material properties and how the interpolation should proceed.

1 Choose **Physics>Subdomain Settings**. On the **Coefficients** page, enter the settings in the table below.

TERM	SUBDOMAIN 1	SUBDOMAIN 2
Constitutive relation	User defined	User defined
θ_s	0.339	0.399
θ_r	0.0001	0.0001
Storage term	User defined	User defined
S	1e-8	1e-8
K_S	0.454	0.298
ρ_f	1000	1000

2 Click the **User Defined** tab and enter these settings, being sure to click **Apply** after you have finished changing the values for each subdomain.

TERM	SUBDOMAIN 1	SUBDOMAIN 2
θ	th_sub1(Hp_esvr[1/m])	th_sub2(Hp_esvr[1/m])
k_r	K_sub1(Hp_esvr[1/m])/0.454	K_sub2(Hp_esvr[1/m])/0.298

3 Click the **Init** tab. In the **Subdomain selection** list, choose both subdomains simultaneously. Then enter the following expression in the **Initial value** edit field and, when done, click **OK**.

INITIAL VALUE	SUBDOMAINS 1, 2
$Hp(t_0)$	-(z+1.2)*(z<-0.4)+(-(z+1.2)-0.2*(z+0.4))*(-0.4<=z)

Boundary Conditions

From the **Physics** menu choose **Boundary Settings**. Set the following conditions; when done, click **OK**.

CONDITION	VARIABLE	BOUNDARY	EXPRESSION
Pressure head	`Hp0`	5	`0.01`
Inward flux	`N0`	2	`-0.454/100`
Zero flux/Symmetry		1,3,4,6–8	

MESH GENERATION

1 Choose **Mesh>Free Mesh Parameters**.

2 On the **Global** page, set the **Predefined mesh sizes** to **Finer**.

3 On the **Boundary** page, select Boundary 4. In the **Maximum element size** edit field, enter `0.02`.

4 Select Boundary 5. In the **Maximum element size** edit field, enter `0.002`.

5 Select Boundary 6. In the **Maximum element size** edit field, enter `0.02`.

6 Click **OK**.

COMPUTING THE SOLUTION

1 From the **Solve** menu, open the **Solver Parameters** dialog box. In the **Solver** list, choose **Time dependent** if it is not already selected.

2 In the **Times** edit field, enter `0:0.05:0.25,0.25:0.25:1,2:1:10`, to generate outputs at 0.05-day increments for 0.25 days, then 0.25-day increments until the end of day 1, and finally 1-day increments through day 10. Click **OK**.

3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 2-39 on page 122, follow these steps:

1 From the **Postprocessing** menu select **Plot Parameters**.

2 Click the **General** tab. In the **Plot type** area select the **Surface**, **Contour**, and **Arrow** check boxes. In the **Solution at time** list select `0.3`.

3 Click the **Surface** tab. In the **Expression** edit field enter `Se_esvr`, typing over current information. Note that `Se_esvr` stands for effective saturation (Se) calculated with this application mode (named `esvr`).

4 Select the **Contour** tab. From the **Predefined quantities** list choose **Pressure head**. Select the option button next to the **Vector with isolevels** label, and in the associated

edit field enter `-2:0.1:2`. Go to the **Contour color** area and click the **Uniform color** option button; click the **Color** button and change the color to white, then click **OK**.

5 Click the **Arrow** tab. In the list of **Predefined quantities** select **Velocity field**. Go to the **Arrow positioning** area, then in the **Number of edit points** edit fields for both **r points** and **z points** enter `25`. Go to the **Arrow parameters** area, click the **Color** button, choose white, then click **OK**. Clear the **Auto** check box, then in the associated edit field enter `0.5`.

6 Click **Apply**.

To generate Figure 2-40 on page 122, click the **General** tab, and in the **Solution at time** list select **1**. Click **OK**.

To generate Figure 2-41 on page 123, continue with these steps:

1 Choose **Postprocessing>Cross-Section Plot Parameters**.

2 Click the **Point** tab. In the **Predefined quantities** list select **Pressure head**. Go to the **Coordinates** area; in the **r** edit field enter `0.2 0.6 1`, and in the **z** edit field enter `-0.1 -0.4 -0.7`. Click **OK**. You should now see a pop-up window designated **Figure 1**; do not close this window.

   To add results from a simulation with the van Genuchten analytic formulas proceed as follows:

3 Choose **Physics>Subdomain Settings**. On the **Coefficients** page go to the **Subdomain selection** list and choose both **1** and **2**. Find the **Constitutive relation** list and select **van Genuchten**.

4 Click the **van Genuchten** tab, then enter the following settings:

TERM	SUBDOMAIN 1	SUBDOMAIN 2
α	1.39	1.74
n	1.6	1.38
l	0.5	0.5

5 Click the **Solve** button on the Main toolbar.

6 When the simulation is finished, return to the **Postprocessing>Cross-Section Plot Parameters** dialog box, click the **General** tab, then select the **Keep current plot** check box. Go to the **Plot in** list and select **Figure 1**. Then click the **Point** tab, click the **Line settings** button, and in the **Line style** list select **Dashed line**; click **OK**, then click **OK**.

Two-Phase Flow

The following example analyzes two-phase flow in porous media. Describing how fluids that do not mix then move simultaneously through one pore space is key to answering many environmental and industrial questions. Unfortunately, multiphase analyses are complicated by the need to solve for multiple dependent variables along with a variety of unknowns. Among them are hydraulic properties that depend on the pressure and saturation levels of each fluid phase.

This problem demonstrates two-phase flow following a U.S. Environmental Protection Agency experimental setup (Ref. 1). This straightforward experiment matches observations for a laboratory column to numerical estimates of two-phase flow. With these column experiments, the researchers evaluate flow for varying fluid pairs (air-water, air-oil, and oil-water) and then match the experimental results to those from computer simulations that employ analytic expressions for retention and permeability. This discussion addresses their work for the Lincoln soil and use formulas from Mualem (Ref. 2) and van Genuchten (Ref. 3) to give hydraulic properties.

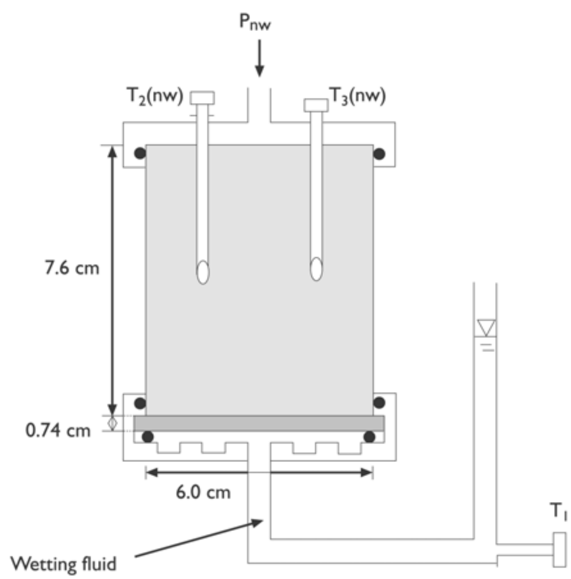


Figure 2-42: Geometry of the two-phase flow column experiments in Hopmans and others (Ref. 1).

This is a multipart example. The first part sets up the two-phase flow model for water and air; the equations solve for pressures. Saturation varies with the solution. An underlying assumption is that at least some residual air and water exist throughout the soil column at all times. The model tracks the gas front as it displaces a wetting fluid by observing saturation rather than assuming a discrete interface. The second part modifies the air-water simulation for air-oil and oil-water systems.

Model Definition

In the experimental setup for air and water, the experiment injects air over the surface of a laboratory column filled with water and sand. The incoming air (the nonwetting phase for this fluid pair) forces the water (the wetting phase) toward the outlet at the base of the column. At the inlet, air pressure increases by steps in time, and no water exits through the column top. In moving to the outlet, the water passes through a disc that is impermeable to air flow. Neither the air nor the water can pass through the vertical column walls. The water pressure at the outlet, which changes in time, corresponds to the height of fluid rise in a receiving buret. The column has a total length of 8.34 cm, a 6-cm radius, and the disk is 0.74 cm thick. The experiment covers 170 hours.

This discussion lays out the two-phase flow simulation in the following order. First it reviews the governing equations and the analytic relationships (Ref. 2 and Ref. 3) that define fluid retention and permeability. Next comes a few implementation details and a table of the model data. The results follow. Finally come step-by-step instructions to build the model in the graphical user interface.

GOVERNING EQUATIONS AND BOUNDARY CONDITIONS

Two-phase flow in porous media follows separate equations for the wetting (w) and nonwetting (nw) fluids:

$$\theta_s \frac{\partial \mathrm{Se}_{\mathrm{w}}}{\partial t} + \nabla \cdot \left[-\frac{\kappa_{\mathrm{int}} k_{r,\,\mathrm{w}}}{\eta_{\mathrm{w}}} \nabla (p_{\mathrm{w}} + \rho_{\mathrm{w}} g D) \right] = 0 \qquad \text{(2-4)}$$

$$\theta_s \frac{\partial \mathrm{Se}_{\mathrm{nw}}}{\partial t} + \nabla \cdot \left[-\frac{\kappa_{\mathrm{int}} k_{r,\,\mathrm{nw}}}{\eta_{\mathrm{nw}}} \nabla (p_{\mathrm{nw}} + \rho_{\mathrm{nw}} g D) \right] = 0 \qquad \text{(2-5)}$$

where θ_s is the total porosity or saturated volume fraction; Se is effective saturation function; t is time (s); κ_{int} is the intrinsic permeability of the porous medium (m^2); k_r is the relative permeability function for a given fluid; η is the fluid's dynamic viscosity (kg/(m·s)); p is pressure (kg/(m·s^2)); ρ is the fluid density (kg/m^3); g is acceleration of gravity; and D is the coordinate (for example, x, y, or z) of vertical elevation (m).

If the fluid distribution is continuous, neither fluid ever completely fills the soil, giving a volume fraction for the wetting phase, θ_{w}, and nonwetting phase, θ_{nw}, at all times. For the wetting phase, θ varies from zero or a small residual value θ_r to the total porosity, θ_s. The effective saturation, Se, comes from scaling θ with respect to θ_s and θ_r and so varies from 0 to 1. Both θ and Se are functions of the pressures of all fluids in the system. You define capillary pressure:

$$p_c = p_{\mathrm{nw}} - p_{\mathrm{w}} \,. \tag{2-6}$$

The pore space can be completely filled with one fluid at a given time:

$$\mathrm{Se}_{\mathrm{w}} + \mathrm{Se}_{\mathrm{nw}} = 1 \,. \tag{2-7}$$

How effective saturation changes with capillary pressure, therefore, is

$$C_{p,\,\mathrm{w}} = -C_{p,\,\mathrm{nw}} = \theta_s \frac{\partial \mathrm{Se}_{\mathrm{w}}}{\partial p_c} \tag{2-8}$$

where C is the specific capacity, and the subscript "p" denotes units of pressure.

Using Equation 2-6, Equation 2-7, and Equation 2-8 in Equation 2-4 and Equation 2-5 simplifies the numerical model. The governing equations become:

$$C_{p,\,\mathrm{w}} \frac{\partial}{\partial t}(p_{\mathrm{nw}} - p_{\mathrm{w}}) + \nabla \cdot \left[-\frac{\kappa_{\mathrm{int}} k_{r,\,\mathrm{w}}}{\eta_{\mathrm{w}}} \nabla (p_{\mathrm{w}} + \rho_{\mathrm{w}} g D) \right] = 0 \tag{2-9}$$

$$-C_{p,\,\mathrm{w}} \frac{\partial}{\partial t}(p_{\mathrm{nw}} - p_{\mathrm{w}}) + \nabla \cdot \left[-\frac{\kappa_{\mathrm{int}} k_{r,\,\mathrm{nw}}}{\eta_{\mathrm{nw}}} \nabla (p_{\mathrm{nw}} + \rho_{\mathrm{nw}} g D) \right] = 0 \,. \tag{2-10}$$

You can solve this system of equations simultaneously for p_{w} and p_{nw}. In this example, the two fluids are incompressible, but that need not be the case.

Initially, the water and air in the column follow hydrostatic distributions. The boundary conditions allow the water to exit only from the base of the soil column. For the wetting phase, the boundary conditions are

$$
\begin{aligned}
&\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p_{\mathrm{w}}+\rho_{\mathrm{w}}gD)\right]=0 && \partial\Omega\ \text{Inlet}\\
&\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p_{\mathrm{w}}+\rho_{\mathrm{w}}gD)\right]=0 && \partial\Omega\ \text{Sides}\\
&p_{\mathrm{w}}=p_{\mathrm{w0}}(t) && \partial\Omega\ \text{Base}
\end{aligned}
\qquad (2\text{-}11)
$$

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

Because air enters at the column top but never exits, the boundary conditions for the nonwetting phase are

$$
\begin{aligned}
&\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p_{\mathrm{nw}}+\rho_{\mathrm{nw}}gD)\right]=0 && \partial\Omega\ \text{Surface}\\
&\mathbf{n}\cdot\left[-\frac{\kappa}{\eta}\nabla(p_{\mathrm{nw}}+\rho_{\mathrm{nw}}gD)\right]=0 && \partial\Omega\ \text{Sides}\\
&p_{\mathrm{nw}}=p_{\mathrm{nw0}}(t) && \partial\Omega\ \text{Base}
\end{aligned}
\qquad (2\text{-}12)
$$

RETENTION AND PERMEABILITY RELATIONSHIPS

You can set up this two-phase flow analysis using interpolation from experimental data, arbitrary mathematical formulas, and results from other equations in the model to define how θ, C, Se, k_r and p_c vary simultaneously. The existing model uses retention and permeability relationships from Ref. 2 and Ref. 3 that express changes in θ, C, Se, and k_r as a function of p_c. Because p_c is large and because changes in θ, C, Se, and k_r are small, these expressions transform capillary pressure to the equivalent height of water or capillary pressure head as in $H_c = p_c/(\rho_{\mathrm{water}}g)$. The hydraulic properties relative to the wetting fluid are

$$\theta_w = \begin{cases} \theta_{r,w} + \mathrm{Se}_w(\theta_{s,w} - \theta_{r,w}) & H_c > 0 \\ \theta_{s,w} & H_c \le 0 \end{cases}$$

$$\mathrm{Se}_w = \begin{cases} \dfrac{1}{[1 + |\alpha H_c|^n]^m} & H_c > 0 \\ 1 & H_c \le 0 \end{cases}$$

$$C_w = \begin{cases} \dfrac{\alpha m}{1-m}(\theta_{s,w} - \theta_{r,w})\mathrm{Se}_w^{\frac{1}{m}}\left(1 - \mathrm{Se}_w^{\frac{1}{m}}\right)^m & H_c > 0 \\ 0 & H_c \le 0 \end{cases} \quad . \qquad (2\text{-}13)$$

$$k_{r,w} = \begin{cases} \mathrm{Se}_w^L\left[1 - \left(1 - \mathrm{Se}_w^{\frac{1}{m}}\right)^m\right]^2 & H_c > 0 \\ 1 & H_c \le 0 \end{cases}$$

where α, n, m, and L are the van Genuchten parameters that denote soil characteristics. Note that with two-phase flow, the van Genuchten-Mualem formulas hinge on the value of H_c.

For the nonwetting fluid, the properties

$$\begin{aligned} \theta_{nw} &= \theta_{s,w} - \theta_w \\ \mathrm{Se}_{nw} &= 1 - \mathrm{Se}_w \\ C_{nw} &= -C_w \\ k_{r,nw} &= (1 - \mathrm{Se}_w)^L\left(1 - \mathrm{Se}_w^{\frac{1}{m}}\right)^{m2} \end{aligned} \qquad (2\text{-}14)$$

arise naturally from the definitions for the wetting phase.

DIFFERENT FLUID PAIRS

When switching between air-water, air-oil, and oil-water experiments, the authors used clever scaling with interfacial tensions according to Leverett (Ref. 4). The Leverett scaling adjusts the nonwetting phase pressure at the column top to produce the same volume of wetting fluid outflow at the column bottom regardless of the fluid pair. With Leverett scaling, switching between fluid pairs requires using the correct fluid properties ρ and η for the fluid pair and adjusting the boundary and initial pressures according to

$$\sigma_{\mathrm{aw}}\ p_{c,\,\mathrm{aw}} = \sigma_{\mathrm{aw}}\ p_{c,\,\mathrm{aw}}$$
$$\sigma_{\mathrm{aw}}\ p_{c,\,\mathrm{aw}} = \sigma_{\mathrm{aw}}\ p_{c,\,\mathrm{ao}}$$
$$\sigma_{\mathrm{aw}}\ p_{c,\,\mathrm{aw}} = \sigma_{\mathrm{aw}}\ p_{c,\,\mathrm{ow}}$$

In these equations, σ represents the interfacial tension between the different fluids, and the subscripts denote the fluid pair. These values appear in a table at the end of this section. For example, $\sigma_{\mathrm{ao}}/\sigma_{\mathrm{aw}}$ equals 0.373, and $\sigma_{\mathrm{wo}}/\sigma_{\mathrm{aw}}$ equals 0.534 N/m; further, the first nonwetting phase pressure head (in meters of water) is 0.4 m for the air-water system, 0.1 m for the air-oil system, and 0.2 m for the water-oil system.

Because relative permeability and retention properties for a porous medium depend on the fluid moving through it, switching fluid pairs also requires switching the retention and permeability properties in the model. This requirement can mean inserting new experimental data or adjusting mathematical formulas. In this model, the authors assessed the permeability and retention parameters were assessed by curve fitting to analytic formulas. They adjusted the parameters α, n, κ_s, and θ_r to get the best fit for each fluid. A review of the data tables that follow reveals that the ratios in the α values for the different fluid pairs roughly equals the σ ratios just given.

Implementation: Numerical Differentiation to Estimate C

This example employs analytic expressions to estimate the specific moisture capacity, C. Because C is the slope of the curve q versus H_c, it also is possible to use the COMSOL Multiphysics differentiation operator `pdiff` to define C such as in

$$C_{p,\mathrm{w}}(p_{\mathrm{w}}) = \texttt{pdiff(theta\_w,Hc)}\ \rho_{\mathrm{water}}{}^{-1} g^{-1}.$$

Thus you can write arbitrary expressions or use data for θ. This equation differentiates fluid volume fraction with respect to capillary pressure head. Here you divide by the weight of water to convert the expression for use in equations with dependent variable pressure. The same type of syntax works with the differentiation operator `diff`. The distinction between the two operators is that `diff` recognizes space and time derivatives already defined in COMSOL Multiphysics (for example, p_x, p_y, p_t), whereas `pdiff` is purely symbolic and does not apply the chain rule for dependent variables.

Implementation: Step Change on a Boundary

The following step-by-step instructions define the timing of the stepped nonwetting phase pressures at the inlet by using an interpolation function. Interpolating in COMSOL Multiphysics is straightforward. You open a dialog box in the **Options** menu, set up the table with the times and corresponding pressure heads, assign a name to the interpolation function, and use the name for where the function is needed, here in the **Subdomain Settings** dialog boxes. To activate the functions created, simply enter the function name (for example, `pnw_t`) along with the argument, that is the time t in parenthesis. The command is

```
pnw(t) = Hnw_t(t)*rhowater*g_w
```

The density of water appears in the equation because Ref. 1 defines the boundary pressure as a height of water.

Data

The data used in this model correspond to the air-water experiments for the Lincoln sand as reported in Ref. 1:

VARIABLE	UNITS	DESCRIPTION	EXPRESSION
g_r	m/s^2	Acceleration due to gravity	9.82
ρ_{fw}	kg/m^3	Fluid density, water	1000
η_w	Pa·s	Dynamic viscosity, water	$1\cdot10^{-3}$
ρ_{fg}	kg/m^3	Fluid density, gas	1.28
η_g	Pa·s	Dynamic viscosity, gas	$1.81\cdot10^{-5}$
κ_{int}	m^2	Intrinsic permeability, column	$2.48\cdot10^{-12}$
κ_s	m^2	Permeability, disc	$1.33\cdot10^{-14}$
$q_{s,w}$		Saturated volume fraction, column	0.32
$q_{s,w}$		Saturated volume fraction, disc	0.5
$p_{nw,top}$	m water	Initial nonwetting phase pressure head, inlet	0.2

The van Genuchten parameters for the different fluid pairs are

VARIABLE	UNITS	DESCRIPTION	AIR-WATER	AIR-OIL	OIL-WATER
$q_{r,w}$		Residual volume fraction	0.021	0.00001	0.0072
α	m^{-1}	alpha parameter	1.89	5.29	3.58

VARIABLE	UNITS	DESCRIPTION	AIR-WATER	AIR-OIL	OIL-WATER
n		n parameter, column	2.811	3.002	3.1365
L		L parameter, column	0.5	0.5	0.5
κ_s	m^{-2}	Permeability, disc	$2.48 \cdot 10^{-12}$	$1.09 \cdot 10^{-12}$	$0.94 \cdot 10^{-12}$

Pressure head at the air inlet increments in time according to

PRESSURE HEAD (M WATER)	START TIME (HOURS)
0.4	0
0.6	21.25
0.8	45.25
1.0	69
1.5	93
2	122.5
4	155

At the water outlet, the fluid level in the receiving buret increases linearly in time from 0 m to 0.1 m.

Results

Figure 2-43 shows an early-time snapshot from the COMSOL Multiphysics solution for two-phase flow in a laboratory column. The shading depicts the effective saturation of the nonwetting phase (air), while the arrows give the wetting phase (water) velocities.

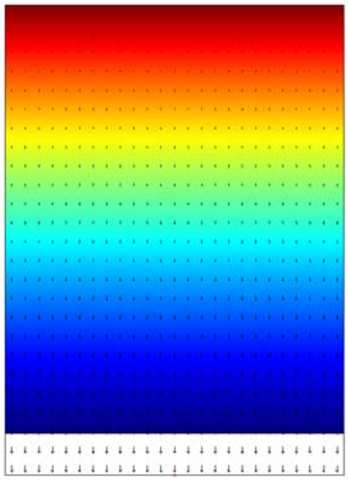


Figure 2-43: Solution to two-phase flow model at 0.1 hours: nonwetting phase saturation (surface plot), wetting-phase velocities (arrows). Results correspond to air-water experiment on Lincoln soil from the US EPA (Ref. 1).

The image illustrates the nonwetting fluid entering the soil column and displacing the wetting fluid. The nonwetting phase enters because it is being forced into the inlet with a multi-step pressure change.

Figure 2-44 shows the stepped pressure head used at the inlet boundary along with the capillary pressure in the column at various elevations. We specified the point locations during postprocessing, which circumvents the need to plan observation sites during input. The solution to the two-phase flow problem provided is an excellent match to the results of Ref. 1.

That the capillary pressure head and the air inlet pressure in Figure 2-44 track together is what made the laboratory setup successful. To get high resolution on the permeability and retention behaviors, the authors in Ref. 1 set the pressure steps large enough that the impact is instantaneous in the soil column. As shown in Figure 2-45, the permeability changes instantaneously throughout the column.

.

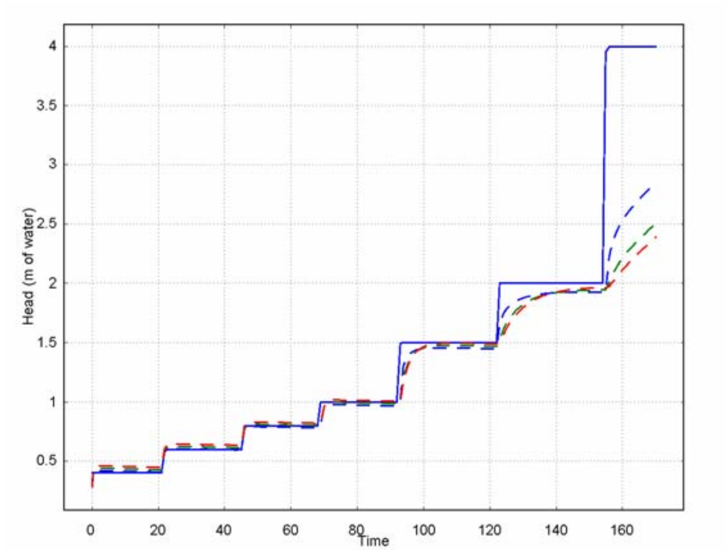


Figure 2-44: Inlet air pressure head (solid lines) and capillary pressure (dashed lines) for air-water flow in Lincoln soil (taken from the US EPA, Ref. 1).

.

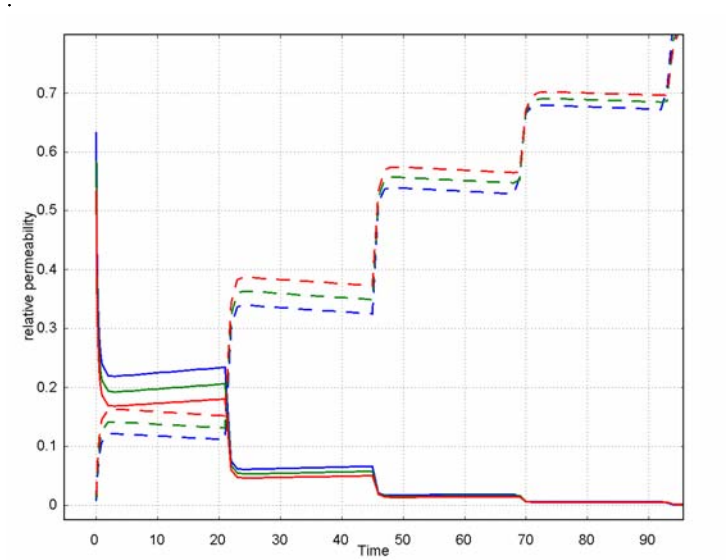


Figure 2-45: Permeability functions for water (solid lines) and air (dashed lines) for Lincoln soil at x = 0.03 m (taken from the US EPA, Ref. 1).

Solutions for two-phase flow for the air-oil and oil-water systems appear in Figure 2-46 and Figure 2-47, respectively.

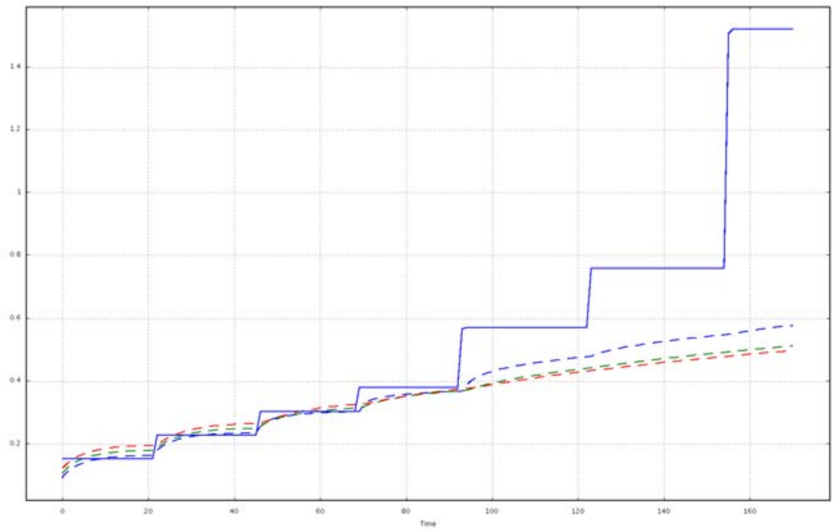


Figure 2-46: Inlet-air pressure head (solid lines) and capillary pressure (dashed lines) for air-oil flow in Lincoln soil (taken from the US EPA, Ref. 1).

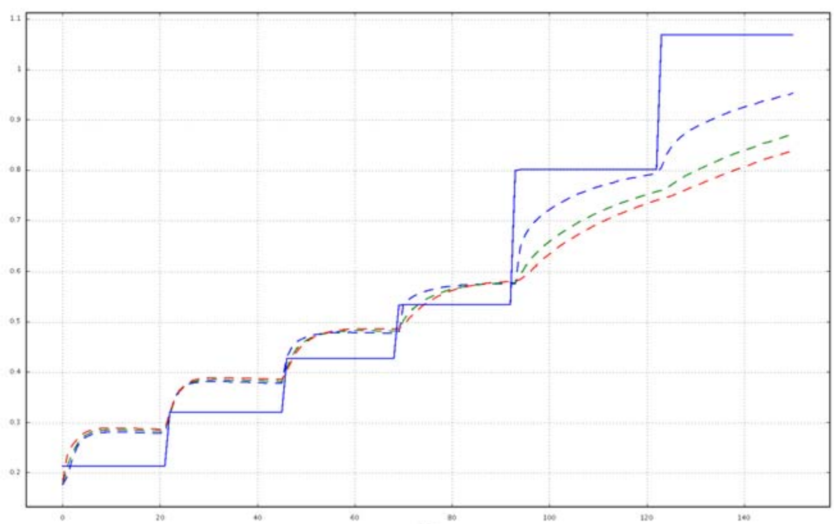


Figure 2-47: Inlet-air pressure head (solid lines) and capillary pressure (dashed lines) for oil-water flow in Lincoln soil. (taken from the US EPA, Ref. 1).

The COMSOL Multiphysics results for the air-oil and oil-water two-phase flow problems prove to be excellent matches to the results shown in Ref. 1. Through Leverett scaling you set the inlet pressure so that the air-oil and oil-water systems would produce the volume outflow rate from the air-water experiment. As with the air-water system, the capillary pressure head and air-inlet pressure for the air-oil experiment track instantaneously. For the water-oil system, however, there is a lag between the nonwetting and wetting phase pressures.

References

1. J.W. Hopmans, M.E. Grismer, J. Chen, and Y.P. Liu, *Parameter estimation of two-fluid capillary pressure saturation and permeability functions*, U.S. Environmental Protection Agency EPA/600/R-98/046, Cincinnati, Ohio, 1998.

2. Y. Mualem, "A new model for predicting the hydraulic permeability of unsaturated porous media," *Water Res. Research*, vol. 12, 1976, pp. 513–522.

3. M.Th. van Genuchten, "A closed-form equation for predicting the hydraulic of conductivity of unsaturated soils," *Soil Sci. Soc. Am. J.*, vol. 44, 1980, pp. 892–898.

4. M.C. Leverett, "Capillary behavior in porous solids," *Trans. AIME*, vol. 142, 1941, pp. 152–169.

Model Library path: `Earth_Science_Module/Fluid_Flow/two_phase_aw`

Modeling Using the Graphical User Interface: Air-Water System

MODEL NAVIGATOR

1. Open the **Model Navigator** to the **New** page, and in the **Space dimension** list select **2D**.
2. From the list of application modes select **Earth Science Module>Fluid Flow>Darcy's Law>Pressure analysis>Transient analysis**.
3. In the **Dependent variables** edit field enter `pw`, and in the **Application mode name** edit field enter `w`.
4. Click the **Multiphysics** button, then click **Add**.
5. In the list of application modes once again select **Earth Science Module>Fluid Flow>Darcy's Law>Pressure analysis>Transient analysis**.

6 Following the procedure you just followed, change the **Dependent variable** to pnw and the **Application mode name** to nw. Click the **Multiphysics** button, then click **Add**.

7 Click **OK**.

GEOMETRY MODELING

Create the geometry by drawing two rectangles.

1 From the **Draw** menu select **Specify Objects>Rectangle**. Enter the following settings; when done, click **OK**.

PARAMETER	VALUE
Width	0.06
Height	0.0074
x	0
z	0

2 Repeat that process except with these settings:

PARAMETER	VALUE
Width	0.06
Height	0.0834
x	0
z	0

3 Click the **Zoom Extents** button on the Main toolbar.

OPTIONS

1 Select the menu item **Options>Constants**, then enter the following names expressions, and descriptions (optional); when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rhowater	1000[kg/m^3]	Density, water
rhow	1000[kg/m^3]	Density, wetting fluid
etaw	0.001*hour[Pa*s]	Dynamic viscosity, wetting fluid
rhonw	1.28[kg/m^3]	Density, nonwetting fluid
etanw	0.0000181*hour[Pa*s]	Dynamic viscosity, nonwetting fluid
hour	3600	

2 From the **Options** menu select **Expressions>Scalar Expressions**. Enter the following names and expressions (they go all on one line); when done, click **OK**.

NAME	EXPRESSION
`pnw_top`	`0.2*rhowater*g_nw`
`pnw_in`	`pnw_top+(.0834-z)*rhonw*g_w`
`pw_in`	`-rhow*g_w*z`
`pw_t`	`0.1*rhowater*g_w/170*t`
`Hc`	`(pnw-pw)/(rhowater*g_w)`
`Sew`	`(1+abs(alpha*Hc)^N)^(-M)*(Hc>0)+1*(Hc<=0)`
`thetaw`	`(thetar+Sew*(thetas-thetar))*(Hc>0)+thetas*(Hc<=0)`
`krw`	`((Sew^L*(1-(1-Sew^(1/M))^M)^2)+eps)*(Hc>0)+1*(Hc<=0)`
`Cp`	`1/rhowater/g_w*((alpha*M/(1-M)*(thetas-thetar)` `*Sew^(1/M)*(1-Sew^(1/M))^M))*(Hc>0)`
`Senw`	`1-Sew`
`thetanw`	`thetas-thetaw`
`krnw`	`((1-Sew)^L*(1-Sew^(1/M))^(2*M))*(Hc>0)+eps`

3 From the **Options** menu select **Expressions>Subdomain Expressions**. Enter the following names and expressions for the two subdomains; when done, click **OK**.

TERM	SUBDOMAIN 1	SUBDOMAIN 2
`thetas`	`0.5`	`0.32`
`thetar`		`0.0211`
`kaps`	`1.34e-14`	`2.48e-12`
`alpha`		`1.89`
`N`		`2.811`
`M`		`1-1/N`
`L`		`0.5`

Now set up the stepped pressures for the nonwetting phase boundary using interpolation.

4 From the **Options** menu select **Functions**.

5 Click the **New** button. In the **Function name** edit field enter `Hpnw_t` and choose the option **Interpolation**. Click **OK**.

6 Enter the following values in the table; when finished, click **OK**:

X	Y
0	0.4
21.20	0.4
21.25	0.6
45.20	0.6
45.25	0.8
68.95	0.8
69	1.0
92.95	1.0
93	1.5
122.45	1.5
122.5	2
154.95	4
155	4
200	4

PHYSICS

In the following stage you first set up the material properties, initial conditions, and boundary conditions for each phase, then link the two equations.

Application Scalar Variables

To set the vertical direction and gravitational constant in the model, go to the **Physics** menu and select **Scalar Variables**. Make the following modifications to the defaults; when done, click **OK**.

NAME	EXPRESSION
D_w	y
g_w	9.82*hour*hour
D_nw	y
g_nw	9.82*hour*hour

This step converts from seconds to days; the quantity is squared because the problem deals with acceleration.

Subdomain Settings—Wetting Phase

1 From the **Multiphysics** menu select **Darcy's Law (w)**.

2 From the **Physics** menu select **Subdomain Settings**. Enter the following settings, then click **Apply**.

TERM	SUBDOMAIN 1	SUBDOMAIN 2
Storage term	User defined	User defined
S	`0`	`Cp`
κ_S	`kaps`	`kaps*krw`
ρ_f	`rhow`	`rhow`
η	`etaw`	`etaw`

3 Click the **Init** tab. Select both Subdomains **1** and **2** simultaneously, and in the **pw(t_0)** edit field for **Pressure** enter `pw_in`. Click **OK**.

Boundary Conditions—Wetting Phase

From **Physics** choose **Boundary Settings**, then set the following conditions; when done, click **OK**.

SETTINGS	BOUNDARY 2	BOUNDARIES 1, 3, 5–7
Boundary condition	Pressure	Zero flux/Symmetry
P_0	`pw_t`	

Subdomain Settings—Nonwetting Phase

1 From the **Multiphysics** menu select **Darcy's Law (nw)**.

2 From the **Physics** menu select **Subdomain Settings**. In the **Subdomain selection** list choose **1**, then clear the **Active in this domain** check box.

3 Select Subdomain 2. Enter the following settings.

TERM	SUBDOMAIN 2
Storage term	User defined
S	`Cp`
κ_S	`kaps*krnw`
ρ_f	`rhonw`
η	`etanw`

4 Click the **Init** tab. Select both Subdomains 1 and 2 simultaneously, and in the **pw(t_0)** edit field for **Pressure** enter `pwn_in`. Click **OK**.

Boundary Conditions—Nonwetting Phase

From the **Physics** menu choose **Boundary Settings**, then set the following conditions; when done, click **OK**.

SETTINGS	BOUNDARIES 1–4, 6, 7	BOUNDARY 5
Boundary condition	Zero flux/Symmetry	Pressure
p_0		`Hpnw_t(t)*rhowater*g_nw`

Equation Systems

1 From the **Physics** menu select **Equation System>Subdomain Settings**.

With the information in this dialog box, COMSOL Multiphysics transforms the inputs you enter to coefficients it uses to solve the finite element model. The box contains entries for each type of model domain: subdomains, boundaries, and points in a 2D problem.

2 Click the $\mathbf{d_a}$ tab. Here is where the coefficients that are multiplied by the time rate change in pressure appear. The 4-element matrix originally has entries on the diagonal: one for the wetting-phase pressure, p_w, for the wetting phase equation; and one for nonwetting phase pressure, p_{nw}, for the nonwetting phase equation. Because the two-phase problem has storage terms for both nonwetting and wetting phases in each equation, you fill in the matrix with the appropriate terms. Modify the matrix so it reads as follows:

PW	PNW
`Cp+eps`	`-Cp+eps`
`-Cp+eps`	`Cp+eps`

Note that `eps` is a very small number.

3 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu select **Free Mesh Parameters**.

2 Click the **Boundary** tab. Using the Ctrl key select both Boundaries 4 and 5. In the **Maximum element size** edit field enter `0.001`.

3 Select Boundary 2, and in the **Maximum element size** edit field enter `0.005`.

4 Click the **Remesh** button.

COMPUTING THE SOLUTION

1. From the **Solver** menu open the **Solver Parameters** dialog box. In the **Solver** list select **Time dependent** (if it is not already selected).
2. In the **Times** edit field enter `0,0:0.01:0.1,0.1:0.1:1,1:170`. Click **OK**.
3. Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 2-43, follow these steps:

1. From the **Postprocessing** menu open the **Plot Parameters** dialog box.
2. In the **Plot type** area select the **Surface**, **Contour**, and **Arrow** check boxes. In the **Solution at time** list choose **0.1**.
3. Click the **Surface** tab, and in the **Expression** edit field enter `Se_nw`, which stands for effective saturation (`Se`) calculated with the application mode named `nw`.
4. Click the **Arrow** tab. In the **Predefined quantities** list select **Darcy's Law (w)> Velocity field**. Go to the **Arrow positioning** area. In the **Number of points** column, and in both the **x points** and **y points** edit fields enter `25`. Go to the **Arrow parameters** area. Click the **Color** button, change the color to black, and click **OK**. Clear the **Auto** check box, and in the **Scale factor** edit field enter `0.5`.
5. Click **OK**.

To generate the plot in Figure 2-44, continue with these steps:

1. From the **Postprocessing** menu open the **Cross-Section Plot Parameters** dialog box.
2. Click the **Point** tab. In the **Expression** edit field enter `Hc`. In the **Coordinates** section, in the **x** edit field enter `0.03 0.03 0.03`, and in the **y** edit field enter `0.02 0.04 0.06`. Click **Apply**.
3. Click the **General** tab. Select the **Keep current plot** check box. In the **Plot in** list select **Figure 1**.
4. Click the **Point** tab. In the **Expression** edit field type `pnw/(rhowater*g_nw)`. In the **Coordinates** area, in the **x** edit field enter `0.03`, and in the **y** edit field enter `0.0834`. Click **OK**.

To generate the plot in Figure 2-45, continue with these steps:

1. From the **Postprocessing** menu open the **Cross-Section Plot Parameters** dialog box.
2. Click the **Point** tab. In the **Expression** edit field enter `kr_w`. In the **Coordinates** section, in the **x** edit field enter `0.03 0.03 0.03`, and in the **y** edit field enter `0.02 0.04 0.06`. Click **Apply**.

3 Click the **General** tab. Select the **Keep Current Plot** check box. In the **Plot in** list select **Figure 1**.
4 Click the **Point** tab. In the **Expression** edit field enter `kr_nw`. Click **OK**.

Two-Phase Flow: Switching Fluid Pairs

This is the second part of the two-phase flow example. Here you modify the air-water model file created in the first part of this example to simulate two-phase flow for the air-oil and oil-water systems discussed in Ref. 1. In the air-oil system, oil is the wetting phase and air is the nonwetting phase. In the oil-water system, water is the wetting phase.

Switching from the air-water system to the air-oil or oil-water systems requires changing the fluid properties and several porous-media parameters. To get the different fluid pairs to produce wetting-phase outflow rates that are similar to those produced with the air-water simulation, you scale the pressure increments at the inlet by interfacial tensions as discussed earlier.

Model Library path: `Earth_Science_Module/Fluid_Flow/two_phase_ao`

Model Library path: `Earth_Science_Module/Fluid_Flow/two_phase_ow`

Modeling Using the Graphical User Interface: Air-Oil and Oil-Water

In the following section you open the file `two_phase_aw.mph` and modify it for the air-oil and oil-water systems. The following tables and instructions describe the changes needed to simulate both two-phase systems.

MODEL NAVIGATOR

Open the **Model Navigator** and click the **Model Library** tab. In the list of library models select **Earth Science Module>Fluid Flow>two_phase_aw**. Click **OK**.

OPTIONS

1 From the **Options** menu open the **Constants** dialog box. Modify the entries for density, viscosity, and add interfacial tensions as in the following table; when finished, click **OK**:

CONSTANT	AIR-OIL	OIL-WATER
rhow	800[kg/m^3]	1000[kg/m^3]
etaw	0.00392*hour[Pa*s]	0.001*hour[Pa*s]
rhonw	1.28[kg/m^3]	800[kg/m^3]
etanw	0.0000181*hour[Pa*s]	0.00392*hour[Pa*s]
sigma_ao	0.0259	
sigma_aw	0.0681	0.0681
sigma_ow		0.0364

2 Open the **Scalar Expressions** dialog box by selecting **Options>Expression**. Enter the following expression. When you are finished, click **OK**.

TERM	AIR-OIL	OIL-WATER
pnw_top	0.2*rhowater*g_nw*sigma_ao/ sigma_aw	0.2*rhowater*g_nw*sigma_ow/ sigma_aw
pw_in	-rhow*g_w*y	-rhow*g_w*z
pw_t	0.1*rhow*g_w/ 170*t*sigma_ow/sigma_aw	0.1*rhow*g_w/150*t

3 Select the menu option **Options>Expressions>Subdomain Expressions**. In the **Subdomain selection** list choose **2**. Change the values for the following expressions; when finished, click **OK**.

NAME	EXPRESSION
kaps	0.94e-12
thetar	0.0072
alpha	3.58
N	3.1365

PHYSICS—NONWETTING

From the **Multiphysics** menu select **Darcy's law (nw)**.

Boundary Conditions—Nonwetting Phase

From the **Physics** menu select **Boundary Settings**. In the **Boundary selection** list choose **5**. Set the following conditions; when done, click **OK**.

BOUNDARY CONDITION	VARIABLE	EXPRESSION
Pressure (for Air/Oil model)	P0	`Hpnw_t(t)* rhowater*g_nw*sigma_ao/sigma_aw`
Pressure (for Oil/Water model)	P0	`Hpnw_t(t)* rhowater*g_w*sigma_ow/sigma_aw`

COMPUTING THE SOLUTION

1 From the **Solver** menu open the **Solver Parameters** dialog box. In the **Solver** list select **Time dependent** (if it is not already selected).

2 Go to the **Time stepping** area. In the **Times** edit field enter `0,0:0.01:0.1,0.1:0.1:1,1:170`. Click **OK**.

3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the plots in Figure 2-47, repeat the steps described for Figure 2-44.

3

Flow and Solid Deformation Models

This chapter contains models with a focus on compaction and poroelasticity.

Compaction and Poroelasticity

Fluids that move through pore spaces in an aquifer or reservoir can shield the porous medium from stress because they bear part of the load from, for instance, overlying rocks, sediments, fluids, and buildings. Withdrawing fluids from the pore space increases the stress the solids bear, sometimes to the degree that the reservoir measurably compacts. The reduction in the pore space loops back and alters the fluid pressures. The feedback brings about more fluid movement, and the cycle continues.

In the Central Valley of California, only a few years of unmanaged pumping irrevocably lowered the ground surface by roughly 9 m and etched out extensive lateral fissures. This model describes the impacts of pumping for a deep basin filled with sediments draping an impervious bedrock step or fault block. That the step is impermeable to fluids is important because the contrast in material properties gives rise to steep pressure gradients and large strains with the potential to produce fissuring or collapse infrastructure elements such as well casings and pipes.

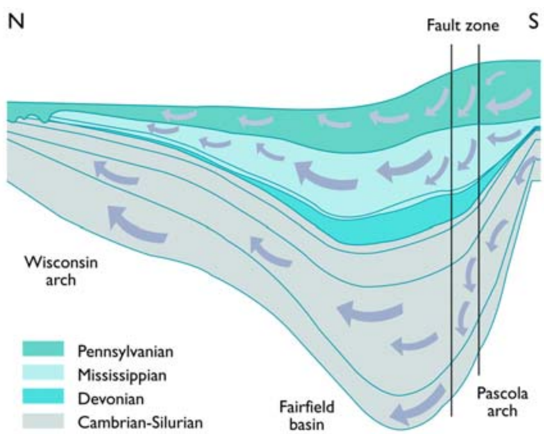


Figure 3-1: Fluid movement in a sedimentary basin with bedrock fault blocks.

This example demonstrates two methods for analyzing ground displacement associated with changing subsurface fluid flow. Both models come directly from the bedrock step problem of Leake and Hsieh (Ref. 1). The first analysis, Terzaghi Compaction, describes a conventional flow model and uses the results in postprocessing to calculate vertical compaction following Terzaghi theory (Ref. 2). The second example, Biot Poroelasticity, models the two-way interaction between the fluid movement and the solid displacement following the linear poroelastic theory of

Biot (Ref. 3). The poroelasticity analysis predicts a similar vertical compaction and also predicts the horizontal displacements that compensate for the change in vertical thickness. The results from poroelastic analyses such as these ones naturally fold into criteria that predict fissuring and compaction at the soil surface as well as failure of wells, pipes, and other infrastructure elements.

Following these two example models, this section shows how to use COMSOL Multiphysics' Darcy's Law application mode and the Plane Strain application mode.

Model Definition

The two models that follow analyze fluid and solid behavior within three sedimentary layers overlying impermeable bedrock in a basin. The bedrock is faulted, which creates a step near a mountain front. The sediment stack totals 420 m at the centerline of the basin ($x = 0$ m) and thins to 120 m above the step ($x > 4000$ m). The top two layers are each 20 m thick.

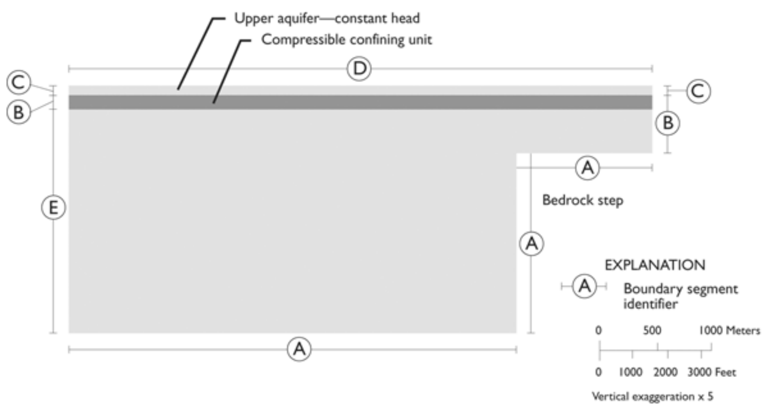


Figure 3-2: Model geometry showing boundary segments (from Leake and Hsieh, Ref. 1).

Pumping from the lower aquifer reduces hydraulic head down the centerline of the basin by 6 m per year. The head drop moves fluid away from the step. The middle layer is relatively impermeable. The pumping does not diminish the supply of fluids in the unpumped reservoir above it. The flow field is initially at steady state. The period of interest is 10 years.

This discussion first covers the Terzaghi Compaction model and follows with the Biot Poroelasticity analysis. Each model description begins with governing equations and boundary conditions followed by particulars related to the COMSOL Multiphysics implementation. A data table comes next, concluding with step-by-step instructions that describe how to build the model in COMSOL Multiphysics.

References

1. S.A. Leake and P.A. Hsieh, *Simulation of Deformation of Sediments from Decline of Ground-Water Levels in an Aquifer Underlain by a Bedrock Step*, U.S. Geological Survey Open File Report 97-47, 1997.

2. K. Terzaghi, *Theoretical Soil Mechanics*, Wiley, 1943, p. 510.

3. M.A. Biot, "Theory of elasticity and consolidation for a porous anisotropic solid," *J. Appl. Phys.*, vol. 26, no. 182, 1955.

4. H.F. Wang, *Theory of Linear Poroelasticity with Application to Geomechanics and Hydrogeology*, Princeton Univ. Press, 2000.

Terzaghi Compaction

Introduction

This example sets up a traditional flow model and analyzes the vertical displacement during postprocessing. The flow field is fully described using the Darcy velocity in an equation of continuity

$$S\frac{\partial H}{\partial t} + \nabla \cdot (-K\nabla H) = 0$$

where S is the storage coefficient (m^{-1}), K equals hydraulic conductivity (m/s), and H represents hydraulic head (m). In most conventional flow models, S represents small changes in fluid volume and pore space in that it combines terms that describe the fluid's compressibility, the solids' compressibility, and the reservoir's porosity. In the original research (Ref. 1) and in this model, S is the compressibility of the solid skeleton, S_{sk}; the original study does not consider fluid compressibility.

Because the aquifer is at equilibrium prior to pumping, you set up this model to predict the change in hydraulic head rather than the hydraulic head values themselves. The main advantage to this approach lies in establishing initial and boundary conditions. Here you specify that the hydraulic head decreases linearly by 60 m over ten years, then simply state that hydraulic head H_0 is zero and remains so where heads do not change in time.

The boundary and initial conditions are

$$\begin{array}{lll l}
\mathbf{n}\cdot K\nabla H = 0 & \partial\Omega & \text{base} & A \\
\mathbf{n}\cdot K\nabla H = 0 & \partial\Omega & \text{other} & B \\
H = H_0 & \partial\Omega & \text{upper edge} & C \\
H = H_0 & \partial\Omega & \text{surface} & D \\
H = H(t) & \partial\Omega & \text{outlet} & E
\end{array}$$

where $\mathbf{n}$ is the normal to the boundary. The letters A through E, taken from Leake and Hsieh (Ref. 1), denote the boundary (see Figure 3-2).

Terzaghi theory uses skeletal specific storage or aquifer compressibility to calculate the vertical compaction Δb (m) of the aquifer sediments in a given representative volume as

$$\Delta b = S_{\mathrm{sk}} b(H_0 - H)$$

where b is standard notation for the vertical thickness of aquifer sediments (m).

Model Data

The following table gives the data for the Terzaghi compaction model:

TABLE 3-1: MODEL DATA

VARIABLE	DESCRIPTION	VALUE
g	Acceleration due to gravity	9.82 m/s^2
ρ_f	Fluid density	1000 kg/m^3
S_{sk}	Skeletal specific storage, aquifer layers	$1 \cdot 10^{-5}\ m^{-1}$
S_{sk}	Skeletal specific storage, confining layer	$1 \cdot 10^{-4}\ m^{-1}$
K_s	Hydraulic conductivity, aquifer layers	25 m/d
K_s	Hydraulic conductivity, confining layer	0.01 m/d
H_0	Initial hydraulic head	0 m
$H(t)$	Declining head boundary	(6 m/year)·t

Results and Discussion

Figure 3-3 shows a Year-10 snapshot from the COMSOL Multiphysics solution to the Terzaghi compaction example. The results describe conventional Darcy flow toward the centering of a basin, moving away from a bedrock step (x > 4000 m). The shading represents the change in hydraulic head brought on by pumping at x = 0 m. The streamlines and arrows denote the direction and magnitude of the fluid velocity. The flow goes from vertical near the surface to horizontal at the outlet. Where the sediments thicken at the edge of the step, the hydraulic gradient and the fluid velocities change abruptly.

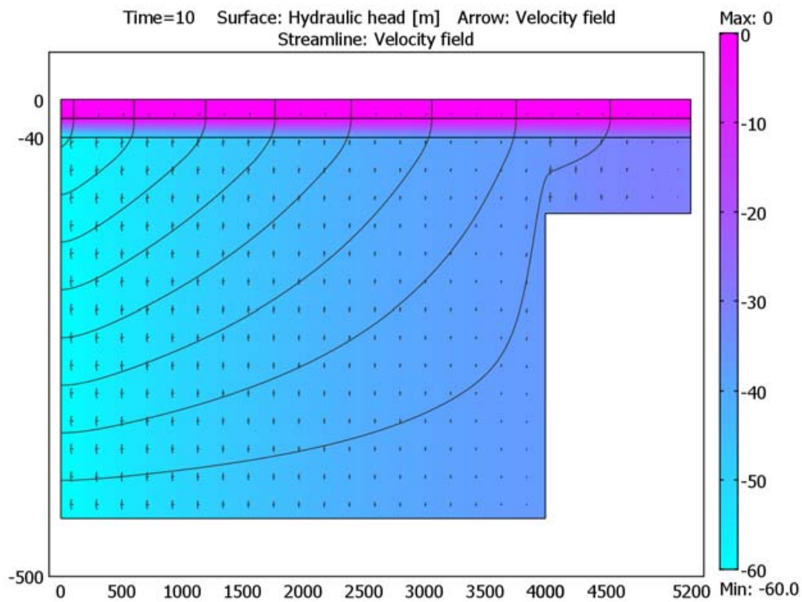


Figure 3-3: COMSOL Multiphysics solution to a Terzaghi flow problem. The figure shows change in hydraulic head (surface plot) and fluid velocity (streamlines and arrows). Note that the vertical axis is expanded for clarity.

Figure 3-4 depicts the vertical compaction predicted for the flow field in Figure 3-3 according to Terzaghi theory. In COMSOL Multiphysics you can define arbitrary expressions that the software evaluates throughout the solution. The vertical-compaction estimates from this analysis are based on such user-defined expressions. The predicted compaction is greatest at the basin centering and declines gradually to the bedrock step. The apparent discontinuity at the step results because the Terzaghi formulas depend linearly on the sediment thickness.

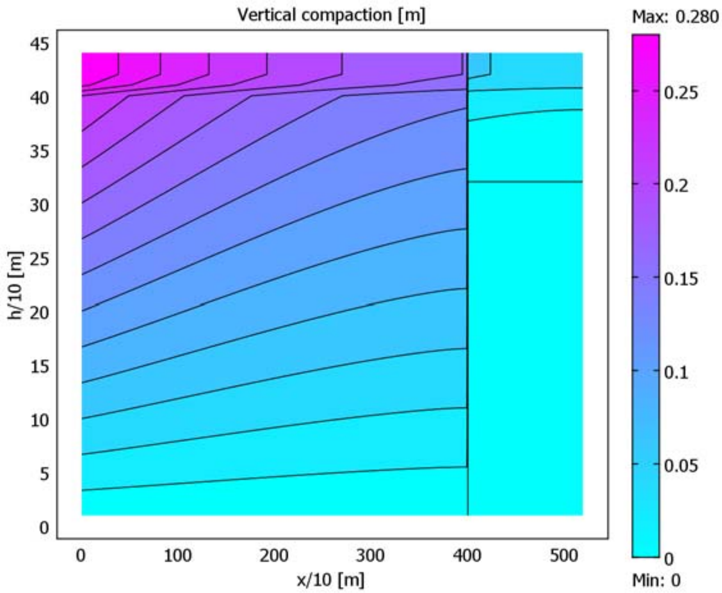


Figure 3-4: Vertical compaction (surface plot and contours) from Terzaghi theory for the Year-10 flow field in Figure 3-3. The vertical axis is expanded for clarity. The coordinate h *denotes the height above the bedrock.*

References

Reference numbers for this model refer to the reference list on page 154.

Model Library path:

`Earth_Science_Module/Flow_and_Deformation/terzaghi_compaction`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

Open the **Model Navigator**. In the list of application modes select **Earth Science Module>Fluid Flow>Darcy's Law>Hydraulic head analysis>Transient analysis**.

GEOMETRY

1 From the **Options** menu select **Axes/Grid Settings**, then click the **Axis** tab. Clear the **Axis equal** check box, and enter the following **x-y limits**:

TERM	EXPRESSION
x min	-100
x max	5300
y min	-500
y max	50

2 Click the **Grid** tab. Clear the **Auto** check box, then enter the following settings; when done, click **OK**.

TERM	EXPRESSION
x spacing	1000
Extra x	4000 5200
y spacing	100
Extra y	-20 -40

3 Choose **Draw>Specify Objects>Rectangle**. Create a rectangle with a **width** of 5200, a **height** of 440, and a **y base** at -440.

4 Follow the same procedure to create another rectangle with a **width** of 1200, a **height** of 320, an **x base** at 4000, and a **y base** at -440.

5 Choose **Draw>Create Composite Object**. In the **Set formula** edit field, type R1-R2, then click **OK**.

6 Click the **Zoom Extents** button on the Main toolbar.

7 Create a break between the layers by adding lines across the rectangle. Go to the Draw toolbar on the left of the COMSOL Multiphysics user interface and click the **Line** symbol. Draw a line across the rectangle at $y = -40$; right-click to end the line. Draw another line across the rectangle at $y = -20$.

OPTIONS AND SETTINGS

Constants

Choose **Options>Constants** and enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho_f	1000[kg/m^3]	Fluid density
SPY	1[year/s]	Seconds per year

The constant SPY is useful for changing the time unit for the model from the default unit second to the more convenient unit year, as you do in this model. This means that wherever the user interface displays seconds, you should read years instead.

Subdomain Expressions

Next define expressions for the skeletal specific storage, S_{sk}, and the hydraulic conductivity, K_s.

Choose **Options>Expressions>Subdomain Expressions** and enter the following names and expressions for the designated subdomains; when done, click **OK**.

NAME	SUBDOMAINS 1, 3	SUBDOMAIN 2
S_sk	1e-5	1e-4
K_s	25*365	0.01*365

The factor 365 in the expressions for the hydraulic conductivity gives this property in the unit m/year (see Table 3-1).

PHYSICS

Application Scalar Variables

Because the gravity constant, g, contains the dimension time, you need to change the value of the corresponding application mode variable, **g_esdl** to convert the effective time unit to years.

1. Choose **Physics>Scalar Variables**.
2. In the **Expression** edit field for **g_esdl**, type `9.82*[m/s^2]*SPY^2`. This gives a gravity constant expressed in m/year^2.
3. In the **Expression** edit field for **Elevation/vertical axis**, type `y`.
4. Click **OK**.

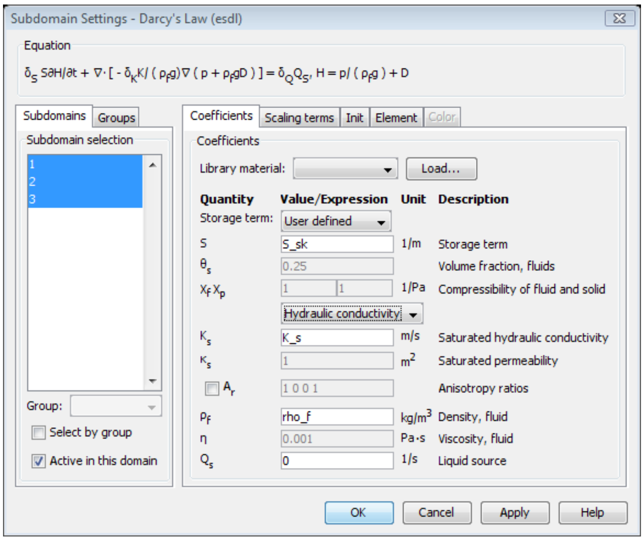
Model Settings

Choose **Physics>Model Settings**. Clear the **Simplify expressions** check box, then click **OK**.

Subdomain Settings

1 Choose **Physics>Subdomain Settings**.

2 Select all three subdomains, then enter data according to the table below.

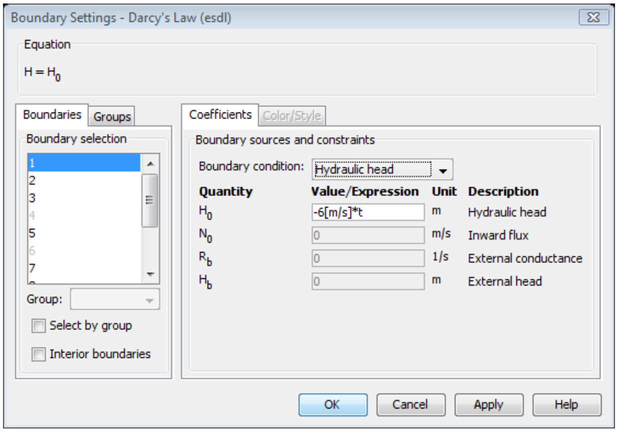


QUANTITY	SELECTION/DESCRIPTION	VALUE
S	User defined	S_sk
K_s	Hydraulic conductivity	K_s
ρ_f	Density, liquid	rho_f

Because the default initial condition is zero, you need not specify it explicitly.

3 From the **Physics** menu, select **Boundary Settings**.

4 Specify boundary conditions according to the table below.



SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3, 8–11	BOUNDARIES 5, 7, 12
Boundary condition	Hydraulic head	Zero flow/Symmetry	Hydraulic head
H_0	`-6[m/s]*t`	-	0

In the expression for H_0 on Boundary 1 (the outlet), the rate of decline in hydraulic head is 6 m/year, but because of the time-unit rescaling you enter seconds instead of years. (If you leave out the unit bracket, you get a warning message but the result will still be correct because the numerical constant is specified so that the resulting expression has the unit displayed to the right of the edit field.)

5 Click **OK**.

MESH GENERATION

Click the **Initialize Mesh** button on the Main toolbar to generate a mesh with the default settings.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 On the **General** page, go to the **Time stepping** area and in the **Times** edit field type `0:1:10`.

Because the effective time unit for the model is 1 year, the above setting instructs COMSOL Multiphysics to compute the solution for years 0 to 10 in 1-year intervals.

3 Click **OK**, then click the **Solve** button on the Main toolbar.

POSTPROCESSING

To generate Figure 3-3 on page 157, proceed as follows:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, verify that the selection in the **Solution at time** list is **10**. In the **Plot type** area, select the **Surface**, **Arrow**, and **Streamlines** check boxes. Clear all the others except for **Geometry edges**.
3. Click the **Surface** tab. On the **Surface Data** page, find the **Predefined quantities** list and select **Hydraulic head**.
4. Click the **Range** button. Clear the **Auto** check box, then click **OK**. This step keeps the current range when plotting earlier time steps.
5. In the **Surface color** area, select **cool** from the **Colormap** list.
6. Click the **Streamline** tab.
7. Go to the **Streamline Data** page, and in the **Predefined quantities** list select **Velocity field**. On the **Start Points** page, click the **Specify start point coordinates** option button. In the **x** edit field, type `0`, and in the **y** edit field, type `-450:50:-50`.
8. At the bottom of the **Streamline** page, click the **Advanced** button. In the **Maximum number of integration steps** edit field, type `10000`, and in the **Stationary point stop tolerance** edit field, type `1e-5`. Click **OK**.
9. Click the **Line Color** tab, then click the **Color** button. In the **Streamline Color** dialog box, select an appropriate color, then click **OK**.
10. Click the **Arrow** tab. Go to the **Arrow Data** page, and in the **Predefined quantities** list choose **Velocity field**. In the **Number of points** edit fields for **x** and **y** enter `25` and `15`, respectively. Go to the **Arrow parameters** area. Clear the **Auto** check box for the **Scale factor**, then in the associated edit field type `0.2`.
11. Click the **Color** button. In the **Arrow Color** dialog box, select an appropriate color, then click **OK**.
12. Click **Apply** to generate the plot.

    To animate all the time steps, proceed with the following instructions:
13. Click the **Animate** tab. In the **Movie settings** area, change the resolution as desired, then click **Start Animation**.
14. Click **OK** to close the **Plot Parameters** dialog box.

To reproduce Figure 3-4 on page 158 you need COMSOL Script or MATLAB to cumulatively sum the compaction along a vertical column and then contour the results.

To generate the plot, first create a data matrix where each entry represents a square 10 m on a side. Then, cumulatively sum the results going up a column. Finally, contour the cumulative. In more detail, the procedure for this task is as follows:

1. To export the data as a matrix, choose **File>Export>Postprocessing Data**.
2. Click the **Subdomain** tab. In the **Expression** edit field, type `-Ssk*H_esdl*10`. Go to the **Location** area and click the **Regular grid** option button. In the **Regular grid specification** area, find the **x points** edit field and enter `520`; then in the **y points** edit field enter `44`. Now each entry represents the compaction in a thickness of 10 m.
3. Click the **General** tab. For **Solution to use**, select only the final time step, **10**. In the **Export to file** edit field, type the file name `terzaghi.txt`. Click the **Browse** button so you can save it in your COMSOL Script working directory, then click **OK**.

If you are to perform the cumulative sum, all entries must have a numeric value. However, the `terzaghi.txt` file you just created contains headers, and `NaN` (not-a-number) appears where the geometry is not defined, such as at the bedrock step. To remove the headers and replace the `NaN`s with zeros, follow these steps:

1. Open `terzaghi.txt` with a text editor.
2. Delete the first few lines of text down to and including the second comment line beginning with `% Data`.
3. Use the editor's Find/Replace function to replace all instances of `NaN` with a number `0`.
4. Save the file.

To perform the cumulative summation and contour the results proceed as follows:

1. Go to the COMSOL Script command line and enter the following command sequence (for details on the various commands, see the *COMSOL Script User's Guide* or the *COMSOL Script Command Reference*):

   ```
   load terzaghi.txt;
   compact = cumsum(terzaghi);
   contourf(compact,[min(min(compact)):0.02:max(max(compact))])
   colormap('cool'); colorbar; hold on
   contour(compact,[min(min(compact)):0.02:max(max(compact))],'k')
   ```

2. Click the **Edit Plot** button in the figure window and edit the plot title and axis labels to finish the plot.

To save the compaction data in a text file, `compact.txt`, give the following command:

```
save -ascii compact.txt compact
```

Biot Poroelasticity

Poroelastic models describe the linked interaction between fluids and deformation in porous media. The fluids in a reservoir absorb stress, which registers as fluid pressure or equally hydraulic head. For example, if pumping significantly reduces pore fluid pressures, sediments could shift due to the increased load. Because the reduction in the pore space brings about more fluid movement, the reservoir could compact further. It follows that lateral stretching must compensate for the vertical compaction.

The Biot poroelasticity analysis in this example bidirectionally couples the Darcy's Law application mode in the Earth Science Module with the Plane Strain application mode in COMSOL Multiphysics. You also can build the model with the Plane Strain application mode from the Structural Mechanics Module. Unidirectional links between the flow and the solids equations also are possible in COMSOL Multiphysics, as is coupling to other physics such as temperature and solute transport.

The U.S. Geological Survey report of Leake and Hsieh (Ref. 1) inspired the Biot poroelasticity model of flow that produces vertical and horizontal displacements as well as the flow-based Terzaghi vertical compaction study already described (see "Terzaghi Compaction" on page 155). The geometry and model description for both analyses are identical; what changes is the link to the solid deformation.

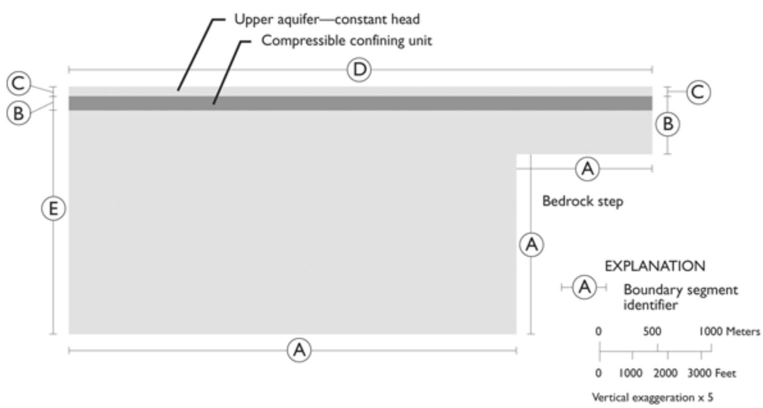


Figure 3-5: Model geometry showing boundary segments (based on Leake and Hsieh, Ref. 1).

Model Definition

Three sedimentary layers overlay impermeable bedrock in a basin where faulting creates a bedrock step near the mountain front. The sediment stack totals 420 m at the deepest point of the basin ($x = 0$ m) but thins to 120 m above the step ($x > 4000$ m). The top two layers of the sequence are each 20 m thick. The first and third layers are aquifers; the middle layer is relatively impermeable to flow. As given by the problem statement, the materials here are homogeneous and isotropic within a layer.

The flow field is initially at steady state, but pumping from the lower aquifer reduces hydraulic head by 6 m per year at the basin center. The head drop moves fluid away from the step. The fluid supply in the upper reservoir is limitless. The period of interest is 10 years.

Governing Equations

Begin the *Biot Poroelasticity* analysis by adding a solids-deformation equation to the *Terzaghi Compaction* model file. Modify the fluid equation to include the time rate change in strain from the solid-deformation equations. Build the solids equation so that it includes the fluid pressure gradient.

FLUID FLOW

Use the Darcy's Law application mode to estimate the flow field in the poroelastic model. The fluid equation is

$$S_{\alpha}\frac{\partial H}{\partial t} + \nabla \cdot [-K\nabla H] = -\alpha_b\frac{\partial}{\partial t}(\nabla \cdot \mathbf{u}) \tag{3-1}$$

where $\frac{\partial}{\partial t}(\nabla \cdot \mathbf{u})$ is the time rate change of strain (s^{-1}) from the equation for solid displacements; and α_b is an empirical constant usually termed the Biot-Willis coefficient. Since $\mathbf{u}$ is a displacement vector (m), the right hand term can be intuitively interpreted as time rate of expansion (divergence) of the solid matrix. The volume fraction available for liquid will increase and thereby give rise to liquid sink, which is why the sign is reversed in the source term. Leake and Hsieh (Ref. 1) defined S_{α} using coefficients from the solids equation, the Young's modulus, E, and Poisson's ratio, ν. For a further discussion about the quantities in the above equation, see the section "Terzaghi Compaction" on page 155 in the Earth Science Module model library. Debate over poroelastic storage coefficients is heated (Ref. 4), and the subscript α here denotes that conventional storage terms might need redefinition for poroelasticity models.

The only differences between the Terzaghi Compaction model already described and this poroelastic analysis lie in material coefficients and sources; the boundary conditions are identical. As in the Terzaghi Compaction model, H is the offset in hydraulic head since an initial steady-state distribution of H_0. This subtle twist simplifies describing the boundary conditions: the value at the outlet boundary becomes the decline in hydraulic head with time, and at the upper aquifer, the hydraulic head is fixed at H_0. All other boundaries have symmetry or no-flow conditions. The boundary and initial conditions for the Darcy's law analysis are

$$
\begin{array}{lll}
\mathbf{n} \cdot K\nabla H = 0 & \partial\Omega \ \text{base} & A \\
\mathbf{n} \cdot K\nabla H = 0 & \partial\Omega \ \text{other} & B \\
H = H_0 & \partial\Omega \ \text{upper edge} & C \\
H = H_0 & \partial\Omega \ \text{surface} & D \\
H = H(t) & \partial\Omega \ \text{outlet} & E
\end{array}
$$

where $\mathbf{n}$ is the normal to the boundary. The letters A through E come from Leake and Hsieh (Ref. 1), each letter denoting a specific boundary (see Figure 3-2).

SOLIDS DEFORMATION

You can define the solids deformation on plane strain. The governing equation in Leake and Hsieh (Ref. 1) is

$$\frac{E}{2(1+\nu)}\nabla^2\mathbf{u} + \frac{E}{2(1+\nu)(1-2\nu)}\nabla \cdot (\nabla\mathbf{u}) = \alpha_b\rho_f g\nabla H \tag{3-2}$$

where E is Young's modulus (kg/(m·d^2)), ν is Poisson's ratio, and $\mathbf{u}$ is the displacement vector composed of orthogonal displacements u and v (m). The term $\alpha_b\rho_f g\nabla H$ (N/m^3) amounts to the fluid pressure gradient in the x and y directions multiplied by the poroelastic constant and is often described as the fluid-to-structure coupling expression. COMSOL Multiphysics efficiently solves the plane-strain problem by converting it to a convenient system of equations as described in the next section.

Parallel to the flow model, the poroelasticity model uses Equation 3-2 to describe change in stresses, σ, strains, ε, and displacement, $\mathbf{u}$, from an initial state. This focus on change in displacement is standard in solids modeling and greatly simplifies specifying loads, boundaries, and initial conditions. For example, a separate body force for gravity need not appear because the changes in load related to the shifting of the water are already described in the coupling term. Moreover, Equation 3-2 defines a state of static equilibrium because the changes in the solid equilibrate quickly, unlike vibrations or waves. Still the time rate of change in strain appears as a coupling term in the poroelastic model because the solids equation becomes quasi-static when solved simultaneously with a time-dependent flow model.

The boundary conditions are a series of constraints on displacement that allow for horizontal movement at the surface and throughout the basin. The base of the sediments is fixed, which means you constrain horizontal and vertical displacement to zero. The upper surface is free to vary in the horizontal and the vertical directions. There is otherwise no horizontal displacement. These conditions result in the following boundary expressions

$u = v = 0$	$\partial\Omega$	base	A
$u = 0$	$\partial\Omega$	other	B
$u = 0$	$\partial\Omega$	upper edge	C
free	$\partial\Omega$	surface	D
$u = 0$	$\partial\Omega$	outlet	E

where, once again, the letters A through E come from Leake and Hsieh, and denote the boundaries in Figure 3-2.

IMPLEMENTATION: PLANE STRAIN APPLICATION MODE

The governing equation for the bedrock step problem describes the deformation state of plane strain, which is the norm for 2D poroelasticity problems (Ref. 1 and Ref. 4). With plane strain, the directional displacements u and v are functions of location in the model plane. The strain, ε, normal to the plane or "into the page" equals zero.

With the Plane Strain application mode, COMSOL Multiphysics solves Equation 3-2 using Navier's equations, a system of expressions that relate stresses, σ, strains, ε, and displacements, **u**, in solids. For equilibrium conditions, the stresses are

$$-\nabla \cdot [\sigma] = \mathbf{F} \qquad (3\text{-}3)$$

where [σ] is the stress tensor, and **F** is the vector that contains the fluid pressure gradient (that is, the fluid-to-structure coupling term) and other body forces when present.

The stress-strain relationship for an isotropic material under plane strain conditions reads

$$\begin{bmatrix}\sigma_x\\\sigma_y\\\tau_{xy}\end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)}\begin{bmatrix}1-\nu & \nu & 0\\ \nu & 1-\nu & 0\\ 0 & 0 & \dfrac{1-2\nu}{2}\end{bmatrix}\begin{bmatrix}\varepsilon_x\\\varepsilon_y\\\gamma_{xy}\end{bmatrix}$$

where τ and γ denote shear stress and shear strain, respectively.

With small deformations, the normal strains ε_{xx}, ε_{yy}, ε_{zz} and shear strains ε_{xy}, ε_{yz}, ε_{xz} relate to the directional displacements u and v for plane strain analyses as follows:

$$\varepsilon_x = \frac{\partial u}{\partial x} \quad \varepsilon_y = \frac{\partial v}{\partial y} \quad \varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \quad \varepsilon_{xy} = \varepsilon_{yx} \qquad \varepsilon_{xz} = \varepsilon_{yz} = \varepsilon_{yz} = 0 \tag{3-4}$$

where strains are defined on directional displacements.

Inserting the relationships from Equation and Equation 3-4 into Equation 3-3 gives the equation that COMSOL Multiphysics solves,

$$-\nabla \cdot (c\nabla\mathbf{u}) = \mathbf{F}$$

where c is a tensor defined on the relationships between stresses, σ, strains, ε, and displacements, $\mathbf{u}$.

Readers curious about the impacts of different assumptions for poroelastic analyses should try switching to one of the time-dependent analyses or even testing large deformations or elastoplastic material laws if working in the Structural Mechanics Module. To find out more about solids analyses, see the section dedicated to Structural Mechanics in the *COMSOL Multiphysics Modeling Guide*, or examine the *Structural Mechanics Module User's Guide* for advanced deformation analysis.

IMPLEMENTATION: TIME RATE CHANGE IN STRAIN

Adding the time rate change in strain to the flow equation is easy using the integral or weak equation form. The weak-form equations are the fundamental form underlying the finite element method of COMSOL Multiphysics and as a results are exceedingly flexible. To find out more about weak formulations see the *COMSOL Multiphysics User's Guide*.

Model Data

The coefficients and parameters for the poroelasticity model are as follows:

VARIABLE	DESCRIPTION	VALUE
g_r	Gravity	9.82 m/s^2
ρ_f	Fluid density	1000 kg/m^3
ρ_s	Solids density	2750 kg/m^3
S_α	Poroelastic storage coefficient, aquifer layers	$1 \cdot 10^{-6}$ m^{-1}
S_α	Poroelastic storage coefficient, confining layer	$1 \cdot 10^{-5}$ m^{-1}
K	Hydraulic conductivity, aquifer layers	25 m/d
K	Hydraulic conductivity, confining layer	0.01 m/d
α	Biot-Willis coefficient	1
H_0	Initial hydraulic head	0 m
$H(t)$	Declining head boundary	(6 m/y)·t
E	Young's modulus, aquifer layers	$8 \cdot 10^8$ N/m
E	Hydraulic conductivity, confining layer	$8 \cdot 10^7$ N/m
ν	Poisson's ratio, all regions	0.25

Results and Discussion

Figure 3-6, Figure 3-7, and Figure 3-8 are Year 2, Year 5, and Year 10 snapshots, respectively, from the COMSOL Multiphysics solution to a well-known problem of linked fluid flow and solid deformation near a bedrock step in a sedimentary basin (Ref. 1). The shading and arrows, respectively, represent the change in hydraulic head and velocities brought about by pumping from the basin interior at x = 0 m. The fluid moves from the surface toward the well screens in the lower aquifer, with an abrupt change in direction and velocity near the bedrock step. In this way, the flow solution here is remarkably similar to the Terzaghi results in Figure 3-3.

The results for the solids displacement tell another story. In Figure 3-6, Figure 3-7, and Figure 3-8, contours and deformed shapes illustrate the total displacement. The plot sequence illustrates the evolution of lateral deformations that compensate for the changing surface elevation above the bedrock step.

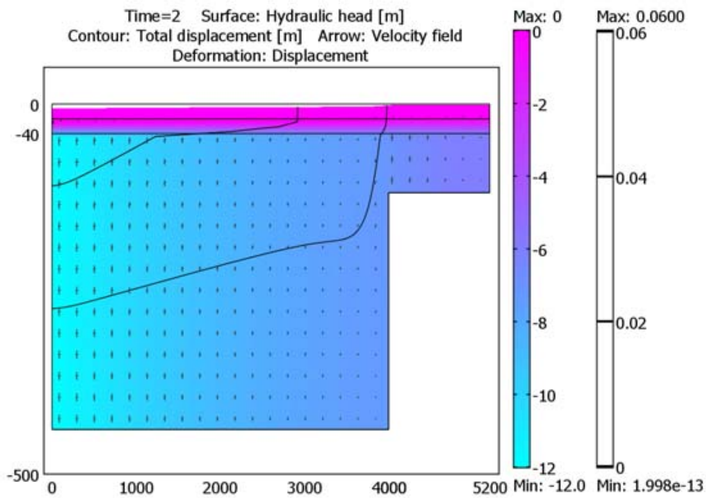


Figure 3-6: Solution for a poroelasticity analysis of the bedrock step problem of Leake and Hsieh (Ref. 1): Hydraulic head (surface plot), displacement (contours and deformations), and fluid velocities (arrows) at Year 2. The vertical axis is expanded for clarity.

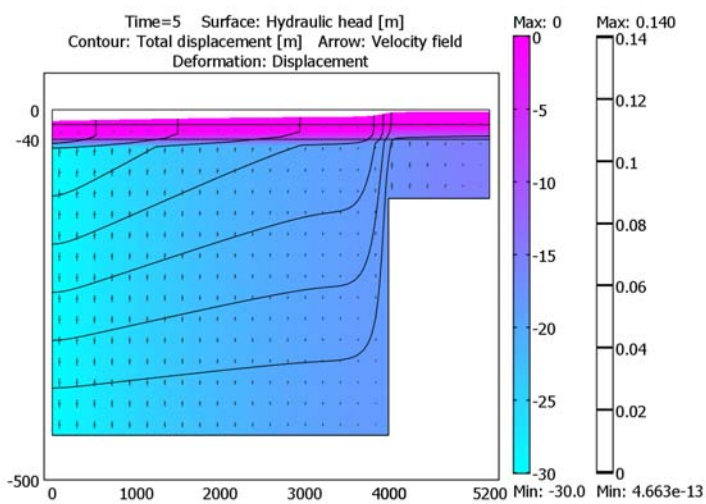


Figure 3-7: Hydraulic head (surface plot), displacement (contours and deformations), and fluid velocities (arrows) at Year 5.

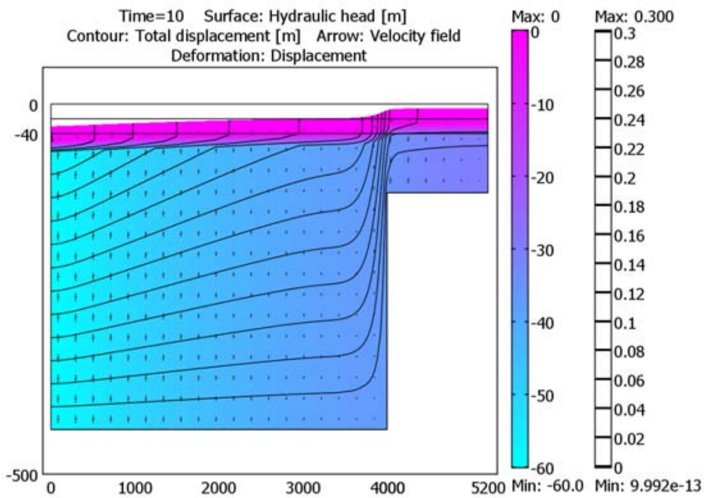


Figure 3-8: Hydraulic head (surface plot), displacement (contours and deformations) and fluid velocities (arrows) at Year 10.

Figure 3-9 directly compares the 10-year solutions from the Biot analysis (dashed lines) and Terzaghi analysis (solid lines). Even at a glance you can notice the similarities in the deep part of the basin as well as the marked departure between the two solutions near the impermeable steep at the mountain front. The results shown here almost perfectly match Figure 3 from Leake and Hsieh (Ref. 1).

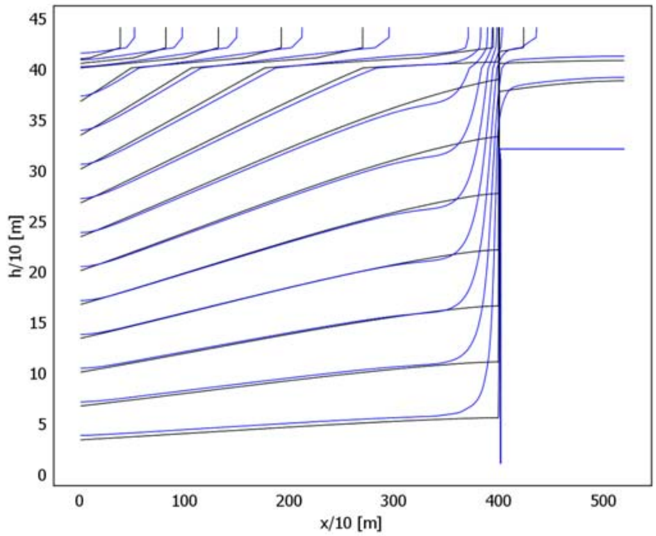


Figure 3-9: COMSOL Multiphysics estimates of displacement from poroelastic analysis (dashed lines) and Terzaghi compaction (solid lines) for the bedrock step problem of Leake and Hsieh (Ref. 1).

In Figure 3-10, streamlines and shading represent the coupling terms that link the fluid and solids equations. The shading gives the time rate of change in strain or the structure-to-fluid link. The streamlines depict the fluid-to-structure couplings that depend on the fluid pressure gradient.

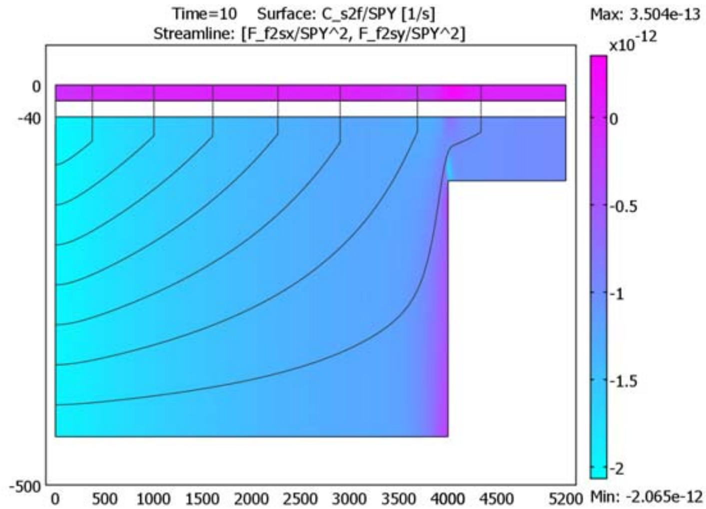


Figure 3-10: The fluid-to-solid (surface plot) and solid-to-fluid (streamlines) coupling terms evaluated at Year 10 with the poroelastic analysis.

The Terzaghi and Biot solutions differ most when it comes to predicting the horizontal strain at the edge of the bedrock step. The Biot poroelasticity analysis predicts horizontal strain; the Terzaghi compaction analysis does not. The horizontal strains at the ground surface from the Biot poroelasticity approach appear in Figure 3-11. It depicts negative strain or compaction immediately on the basin side of the step; the positive strains correspond to tension or lengthening on the mountain side.

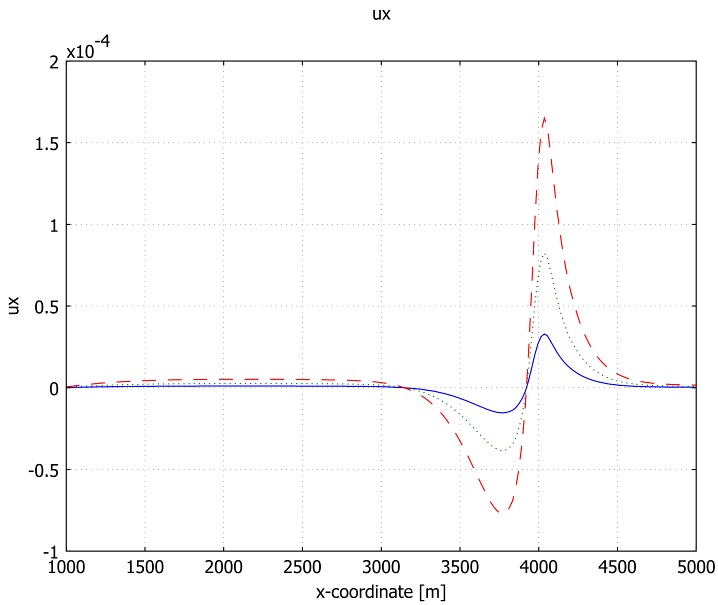


Figure 3-11: COMSOL Multiphysics estimates of horizontal strain from poroelastic analysis for the bedrock step problem of Leake and Hsieh: Year 2 (blue, solid line), Year 5 (green, dotted line), and Year 10 (red, dashed line).

Failure criteria or expressions defining a critical threshold for stress, strain, or displacements facilitate evaluating whether the strain differential at the bedrock steps is big enough to produce fissures. Figure 3-12 plots von Mises stresses (surface plot), fluid velocities (streamlines), and total displacement (deformation). The von Mises stresses are postprocessing variables defined by COMSOL Multiphysics in all structural-deformation analyses. The von Mises stresses are variables in many failure expressions and you can also use them as yield functions in the elasto-plastic materials dialog boxes.

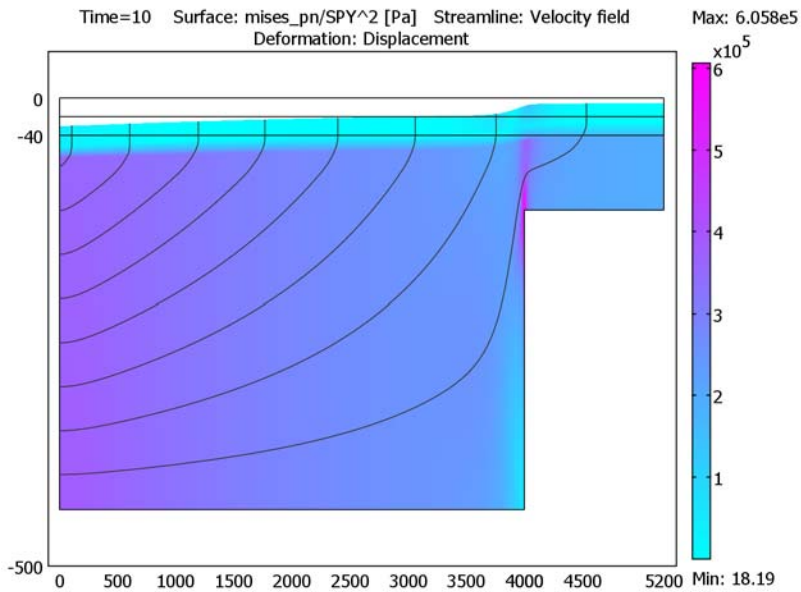


Figure 3-12: COMSOL Multiphysics estimates of von Mises stresses (surface plot), fluid velocities (streamlines), and displacement (deformation) at Year 10. These results correspond to the porelastic analysis from Leake and Hsieh (Ref. 1). The vertical axis and deformation are exaggerated for clarity.

References

Reference numbers for this model refer to the reference list on page 154.

Model Library path: `Earth_Science_Module/Flow_and_Deformation/biot_poroelasticity`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 From the **File** menu, select **Open Model Library**. From the **Model Library** tree, select **Earth Science Module>Flow and Deformation>terzaghi compaction**. Click **OK**.

2 From the **Multiphysics** menu, select **Model Navigator**. In the list of application modes select **COMSOL Multiphysics>Structural Mechanics>Plane Strain**. Click **Add**, then click **OK** to close the **Model Navigator**.

3 From the **Multiphysics** menu, select **Darcy's Law (esdl)** (you set up the flow model before beginning with the solids-deformation problem).

OPTIONS AND SETTINGS

1 Choose **Options>Constants**.

2 Add the following names, expressions, and descriptions (optional) to those already present in the table; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho_s	2750[kg/m^3]	Solids density
alpha_b	1	Biot-Willis coefficient

3 Choose **Options>Expressions>Scalar Expressions**. Enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
F_f2sx	-alpha_b*rho_f*g_esdl*Hx_esdl	Fluid-to-structure coupling expression, x direction
F_f2sy	-alpha_b*rho_f*g_esdl*Hy_esdl	Fluid-to-structure coupling expression, y direction

Here uxt and vyt are the COMSOL Multiphysics variables corresponding to $\partial_t \partial_x u$ and $\partial_t \partial_y v$, respectively.

4 Choose **Options>Expressions>Subdomain Expressions**. Add the following expressions to the table; when done, click **OK**.

NAME	SUBDOMAINS 1, 3	SUBDOMAIN 2
S_alpha	1e-6	1e-5
nu	0.25	0.25
E	800[MPa]*SPY^2	80[MPa]*SPY^2
C_s2f	alpha_b*(uxt+vyt)	

The factor SPY^2 in the expressions for Young's modulus, E, is required for the time-unit conversion from seconds to years because E scales with time, T, as T^{-2}.

The expression C_s2f, is the structure-to-fluid coupling in the fluid equation (Equation 3-1).

PHYSICS

Application Scalar Variables

Choose **Physics>Scalar Variables**. Verify that the gravitational constant **g_esdl** has a value of `9.82[m/s^2]*SPY^2`. When done, click **OK**.

Subdomain Settings

1 Choose **Physics>Subdomain Settings**.

2 In the **Subdomain selection** list, select all three subdomains, then change the entry in the **S** edit field for the storage term to `S_alpha`.

3 In the $\mathbf{Q_s}$ edit field, type `-alpha_b*(uxt+vyt)`. This term defines the right-hand side of Equation 3-1 on page 166.

4 Click **OK** to close the dialog box.

5 Return to the **Multiphysics** menu and select **Plane Strain (pn)**.

6 Choose **Physics>Subdomain Settings**.

7 Go to the **Material** page. In the **Subdomain selection** list select all three subdomains and then enter these settings:

QUANTITY	VALUE/EXPRESSION
E	E
ν	nu
ρ	rho_s

8 Click the **Load** tab, then select all three subdomains. In the $\mathbf{F_x}$ edit field, type `F_f2sx`, and in the $\mathbf{F_y}$ edit field, type `F_f2sy`.

9 Click **OK**.

Boundary Conditions

1 Choose **Physics>Boundary Settings** and then click the **Constraints** tab.

2 In the **Boundary selection** list, choose **1**, **2**, **3**, **5**, and **8**–**12**. Click the **Standard notation** option button, select the $\mathbf{R_x}$ check box, and then in the associated edit field, type `0`.

3 Similarly select boundaries **2**, **8**, and **9**. This time select the $\mathbf{R_y}$ check box, and in the associated edit field type `0`.

Note that the surface and sides of the upper aquifer are free so they need no boundary conditions.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Fine**. Click **OK**.

3 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 The solution time should already be specified for this example. If you want to verify this, the setting in the **Times** edit field in the **Solver Parameters** dialog box should be `0:1:10`, corresponding to a 10-year range divided into 1-year intervals.

2 COMSOL Multiphysics saves old problems and solutions in an M-file. Sometimes they stack up and slow the solution. To clear out the old mesh and solution, choose **File>Reset Model**. In this case, however, the software should solve the problem properly without you needing to clear the memory.

3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING

To generate the plots in Figure 3-6, Figure 3-7, and Figure 3-8, proceed as follows:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select **2** from the **Solution at time** list.

3 In the **Plot type** area, select the **Surface**, **Contour**, **Arrow**, and **Deformed shape** check boxes. Clear the **Streamline** check box.

4 Click the **Surface** tab. On the **Surface Data** page, verify that the selection in the **Predefined quantities** list is **Darcy's Law (esdl)>Hydraulic head**.

5 Click the **Range** button, select the **Auto** check box, and then click **OK**.

6 Click the **Contour** tab. On the **Contour Data** page, select **Plane Strain (pn)>Total displacement** from the **Predefined quantities** list.

7 Go to the **Contour levels** area and in the **Vector with isolevels** edit field, type `0:0.02:0.4`.

8 Click the **Arrow** tab. On the **Subdomain Data** page, verify that the selection in the **Predefined quantities** list is **Darcy's Law (esdl)>Velocity field**. Keep also the other settings imported from the Terzaghi Compaction model.

9 Click the **Deform** tab. From the **Predefined quantities** list on the **Subdomain Data** page, select **Plane Strain (pn)>Displacement**.

10 Clear the **Auto** check box for the **Scale factor**, and in the associated edit field type `100`.

11 Click **Apply** to generate the plot in Figure 3-6.

12 Generate the plots in Figure 3-7 and Figure 3-8 by changing the selection in the **Solution at time** list in Step 2 to **5** and **10**, respectively, and then clicking **Apply**.

To animate all the time steps, do as follows:

1 Back in the **Plot Parameters** dialog box, click the **Animate** tab.

2 In the **Movie settings** area, change the resolution as desired, then click **Start Animation**.

Note: To generate the following figure you must run COMSOL Multiphysics with COMSOL Script or MATLAB.

To generate Figure 3-9 on page 173, contour the Terzaghi compaction estimates in the file `compact.txt` and then overlay the plot of total displacement estimates from the Biot poroelasticity analysis by completing the following steps:

1 Choose **File>Export>Postprocessing Data**.

2 Click the **General** tab. As the **Solution to use**, highlight only the final time step, **10**. Browse to your COMSOL Script working directory and specify the export file name `displacement.txt`.

3 Click the **Subdomain** tab. In the **Expression** edit field, type `-disp_pn` (the negative of the total displacement). In the **Location** area, click the **Regular grid** option button. Locate the **Number of points** column in the **Regular grid specification** area and enter `520` in the **x points** edit field and `44` in the **y points** edit field.

   The resulting file, `displacement.txt`, contains headings, and NaN (not a number) appears where the geometry is not defined. You must clear these items before plotting the data. To do so, open `displacement.txt` in a text editor, delete the upper headers up to and including the line beginning with `% Data`, replace all NaN entries with the number `0`, and then save the file.

4 To contour the compaction and displacement results, go to the COMSOL Script command line; if necessary, change the current working directory to the directory where you saved the data files `compact.txt` (see page 164) and `displacement.txt`; and then enter the following sequence:

```
load compact.txt
load displacement.txt
min_d = min(min(displacement));
max_d = max(max(displacement));
contour(compact,[min_d:0.02:max_d],'k-')
hold on
contour(displacement,[min_d:0.02:max_d],'b--')
```

5 Click the **Edit Plot** button in the figure window and edit the plot title and axis labels to finish the plot.

To generate Figure 3-10 on page 174, perform these steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 In the **Solution at time** list on the **General** page, select the final output time, **10**. In the **Plot type** area select the **Surface**, **Arrow**, and **Streamlines** check boxes. Clear the **Deformed shape** check box.

3 Click the **Surface** tab. On the **Surface Data** page, type `C_s2f/SPY` in the **Expression** edit field. Click the **Range** button, select the **Auto** check box, then click **OK**. Go to the **Surface color** area and make an appropriate selection in the **Colormap** list.

4 Click the **Arrow** tab. On the **Subdomain Data** page, select **Darcy's Law (esdl)>Velocity field** from the **Predefined quantities** list. In the **Arrow positioning** area, enter `25` in the **x points** edit field and `15` in the **y points** edit field. Clear the **Auto** check box for the **Scale factor**, then in the associated edit field type `0.2`.

5 Click the **Streamline** tab. On the **Streamline Data** page, type `F_f2sx/SPY^2` in the **x component** edit field and `F_f2sy/SPY^2` in the **y component** edit field. From the **Streamline plot type** list, select **Start point controlled**. On the **Start Points** page, click the **Specify start point coordinates** option button. In the **x** edit field enter `0`, and in the **y** edit field enter `-450:50:-50`.

6 Click the **Advanced** button at the bottom of the dialog box. In the **Maximum number of integration steps** edit field enter `10000`, then in the **Stationary point stop tolerance** edit field enter `0.00001`. Click **OK**.

7 In the **Streamline color area** click the **Color** button. Choose an appropriate line color, then click **OK**.

8 Finally, click **OK** to close the **Plot Parameters** dialog box and generate the plot.

To reproduce the plot in Figure 3-11 on page 175, continue with these steps:

1 Choose **Postprocessing>Cross-Section Plot Parameters**.

2 On the **General** page, in the **Solutions to use** list select **2**, **5**, and **10**.

3 Click the **Line/Extrusion** tab. Go to the **y-axis data** area and in the **Expression** edit field enter `ux`.

4 In the **x-axis data area**, click the lower option button, then click the **Expression** button. In the **X-Axis Data** dialog box, type `x` in the **Expression** edit field. Click **OK**.

5 In the **Cross-section line data** area, enter data from the following table:

x0	x1	y0	y1
1000	5000	0	0

6 Click **OK**.

Finally, to generate Figure 3-12 on page 176, follow these instructions:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, examine the **Solution at time** list and verify that the final output time **10** is selected. In the **Plot type** area, select the **Surface**, **Arrow**, **Streamline**, and **Deformed shape** check boxes.

3 Click the **Surface** tab. In the **Predefined quantities** list on the **Surface Data** page, select **Plane Strain (pn)>von Mises stress**. Edit the **Expression** field entry so that it reads `mises_pn/SPY^2`. Go to the **Surface color** area and make an appropriate selection in the **Colormap** list.

4 Click the **Streamline** tab. In the **Predefined quantities** list on the **Streamline Data** page, select **Darcy's Law (esdl)>Velocity field**. Accept the previously specified start points.

5 Click the **Arrow** tab. In the **Predefined quantities** list on the **Subdomain Data** page, select **Darcy's Law (esdl)>Velocity field**.

6 Click **OK**.

Open-Hole Multilateral Well—Poroelastic Flow and Deformation

Multilateral wells—those with multiple legs that branch off from a single conduit—can produce oil efficiently because the legs can tap multiple productive zones and navigate around impermeable ones. Unfortunately, drilling engineers must often mechanically stabilize multilateral wells with a liner or casing, which can cost millions of dollars. Leaving the wellbore uncased or "open" reduces construction costs, but it runs a relatively high risk of catastrophic failure both during installation and after pumping begins.

This COMSOL Multiphysics model examines the mechanical stability of an open-hole multilateral well during pumping using poroelastic simulations with Coulomb failure criteria. The data and geometry come from *E-base*, a proprietary database from TerraTek (www.terratek.com) that holds data concerning well and rock mechanics. The model itself builds on theory outlined by Roberto Suarez-Rivera of TerraTek (Ref. 1).

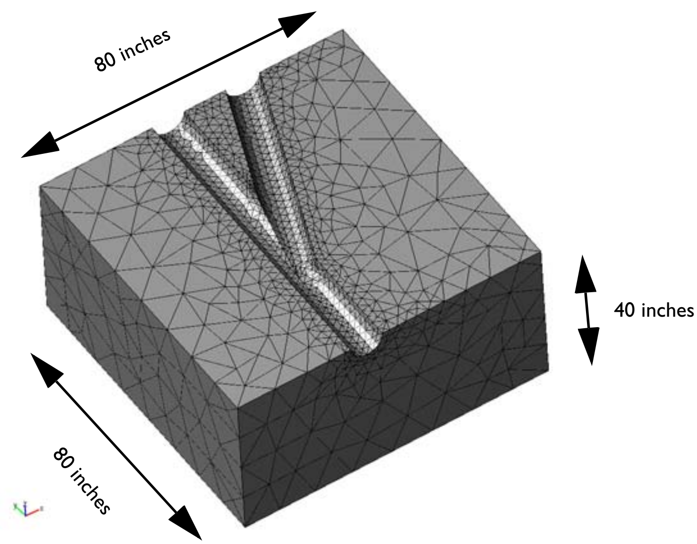


Figure 3-13: Geometry for a COMSOL Multiphysics analysis of a horizontal open-hole multilateral well.

The poroelastic simulations estimate 3D compaction related to pumping by taking subsurface fluid flow with Darcy's law and coupling it to structural displacements with a stress-strain analysis. The simulation results feed into the Coulomb expression that maps where the compaction from the pumping is enough to have the well fail. The discussion in Ref. 1 couples flow and deformation analyses with failure criteria to predict if the well fails both during emplacement and as a result of pumping. This model focuses on elastic displacements brought on by changing fluid pressures when pumping begins. Related analyses for elasto-plastic deformations are straightforward using material laws automated in the Structural Mechanics Module.

Model Definition: Flow and Deformation Simulation

The modeled geometry (Figure 3-13) is the lower half of a branching junction, a segment from a larger well network. The junction lies roughly 25 feet from the start of the well. The entire well network extends much further, perhaps hundreds of feet. The well is 8.5 inches in diameter and sits in a cube 80 inches on each side. Pumps move fluid from the reservoir into the well. Fluid exits the geometry only through the well. The displacement at the reservoir edge is constrained. The walls of the well, however, deform freely. The goal is to solve for the change in fluid pressure, stress, strain, and displacement that the pumping causes rather than their absolute values.

FLUID FLOW

To describe fluid flow, you insert the Darcy velocity into an equation of continuity

$$\nabla \cdot \left[-\frac{\kappa}{\eta}\nabla p\right] = 0$$

where κ is the permeability, η is the viscosity, and p equals the pressure of the oil in the pore space.

For the flow boundaries, you already know the change in fluid pressure from the well to the reservoir edge. The planar surface adjacent to the well (between the upper and lower blocks) is a symmetry boundary. Because the well is the only exit for the fluid, there is no flow to or from connecting well segments. In summary,

$$\begin{array}{ll} p = p_{\mathrm{r}} & \partial\Omega \ \text{reservoir} \\ \mathbf{n}\cdot\left[-\dfrac{\kappa}{\eta}\nabla p\right] = 0 & \partial\Omega \ \text{symmetry face} \\ \mathbf{n}\cdot\left[-\dfrac{\kappa}{\eta}\nabla p\right] = 0 & \partial\Omega \ \text{connecting segments} \\ p = p_{\mathrm{w}} & \partial\Omega \ \text{well} \end{array}$$

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

SOLID DEFORMATION

The system of equations that describes the solids deformation is

$$-\nabla\cdot(c\nabla\mathbf{u}) = \mathbf{F} = \alpha\nabla p$$

where $\mathbf{u}$ is a vector of the directional displacements u, v, and w, and the directional components of the gradient in fluid pressure, p, make up a vector forces, $\mathbf{F}$. The coefficient c relates the displacements to the stresses and the strains in this way:

$$\begin{array}{lll} \varepsilon_x = \dfrac{\partial u}{\partial x} & \varepsilon_{xy} = \dfrac{1}{2}\left(\dfrac{\partial u}{\partial y}+\dfrac{\partial v}{\partial x}\right) & \\ \varepsilon_y = \dfrac{\partial v}{\partial y} & \varepsilon_{yz} = \dfrac{1}{2}\left(\dfrac{\partial v}{\partial z}+\dfrac{\partial w}{\partial y}\right) & \sigma = \begin{bmatrix} \sigma_x & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_y & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_z \end{bmatrix} \\ \varepsilon_z = \dfrac{\partial w}{\partial z} & \varepsilon_{xz} = \dfrac{1}{2}\left(\dfrac{\partial u}{\partial z}+\dfrac{\partial w}{\partial x}\right) & \end{array}$$

where ε is the strain tensor, and σ denotes the stress tensor. The terms ε and σ are related by $\sigma = D\varepsilon$. D, a 36-entry tensor, is a function of Young's modulus, E, and Poisson's ratio, ν.

For the boundary conditions, the model constrains movement at all external boundaries. The well opening is free to deform. In summary:

$$\begin{array}{ll} u = v = w = 0 & \partial\Omega \ \text{reservoir} \\ w = 0 & \partial\Omega \ \text{symmetry face} \\ v = 0 & \partial\Omega \ \text{connecting segments} \\ \text{free} & \partial\Omega \ \text{well} \end{array} .$$

Results: Flow and Deformation Simulation

The following figures show results from simulations for coupled fluid flow and reservoir deformation following a poroelastic approach for the horizontal multilateral well reported in Ref. 1.

The isosurfaces in Figure 3-14 indicate the fluid pressure throughout the well's lower half. The streamlines show the fluid paths and velocities. Fluid pressure drops from the reservoir toward the well opening. The velocity typically increases toward the well but remains close to zero near the branching legs of the junction.

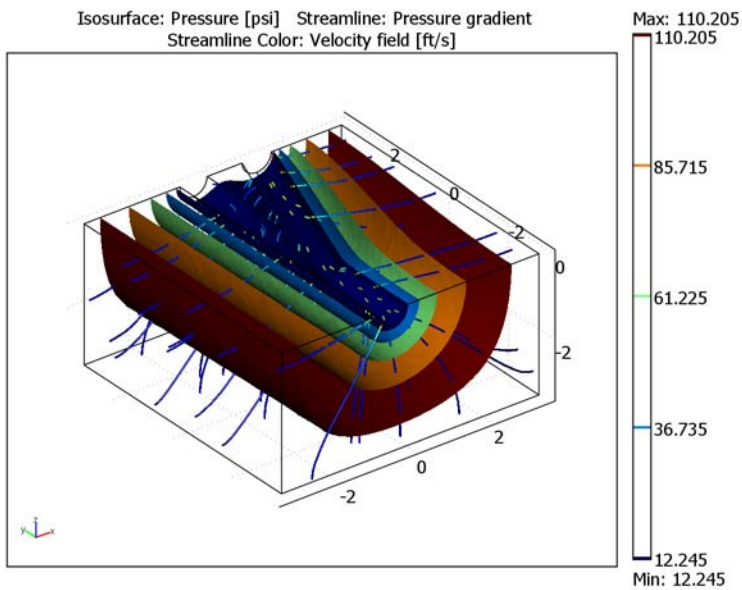


Figure 3-14: COMSOL Multiphysics poroelastic analysis of a multilateral well. Results are fluid pressure (the isosurfaces), pressure gradient (streamlines), and fluid velocities (streamline shading).

Results for elastic deformation appear in Figure 3-15. The surface shading denotes total displacement. The plot illustrates directional displacements by shifting the shading relative to an outline of the original geometry. For a clear view, the displacements are exaggerated. The uncased surface yields slightly because the deformed shading fills in the hollows of the well. The largest displacements occur just above the split in the well.

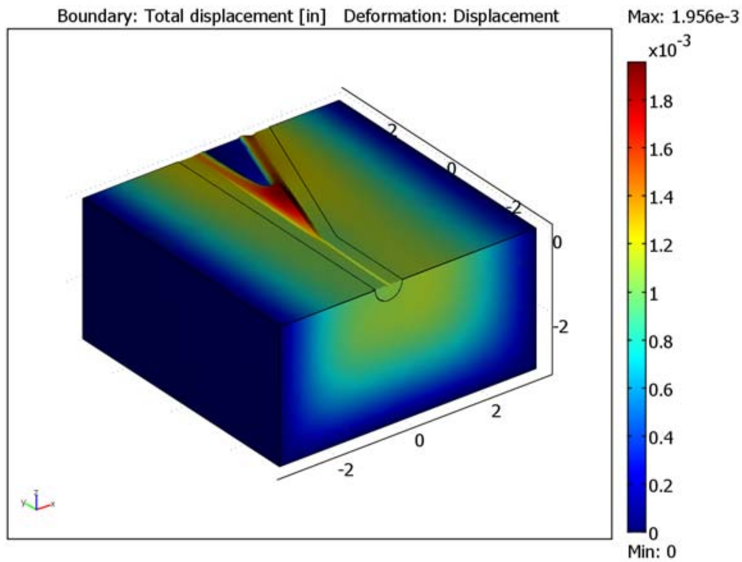


Figure 3-15: COMSOL Multiphysics estimates of displacement. Shading indicates the total displacement, and the geometry appears as lines. Even as the deformed shape shifts, those lines remain steady; the shaded image shows movement relative to the geometry outlines.

Figure 3-16 plots the pressure isosurfaces and the velocity streamlines from Figure 3-14 with the displacements from Figure 3-15 using wire-mesh options directly available from the COMSOL Multiphysics postprocessing user interface.

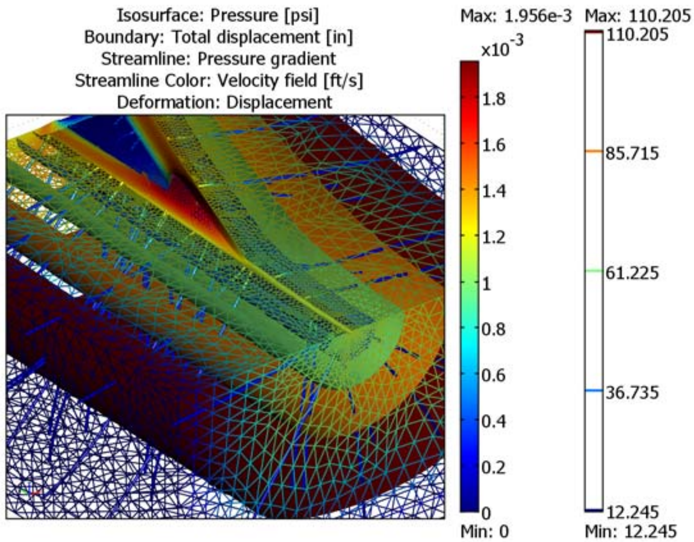


Figure 3-16: Poroelastic analysis near a branch in a multilateral well showing fluid pressures (the isosurfaces), velocity (streamtubes), total displacement (the mesh), and directional displacements (the deformed shape).

Failure Criterion

This model allows the evaluation of failures during postprocessing using results from the fluid-flow and solid-deformation simulations shown in the preceding figures. This discussion follows calculations that Ref. 1 uses to map calculations indicating where pumping could compact the reservoir enough (see Figure 3-15) that the well will fail. Refer to Ref. 1 to estimate the critical rock strength required to successfully emplace the well, and also to learn more about calibration to data.

The 3D Coulomb failure criterion in Ref. 1 relates rock failure, the three principal stresses (σ_1, σ_2, and σ_3), and the fluid pressures as follows:

$$\begin{aligned} \text{fail} &= (\sigma_3 + p) - Q(\sigma_1 + p) + N\left(1 + \frac{(\sigma_2 - \sigma_1)}{(\sigma_3 - \sigma_1)}\right) \\ Q &= \frac{1 + \sin\phi}{1 - \sin\phi}, \qquad N = \frac{2\cos\phi}{1 - \sin\phi}\mathrm{So} \end{aligned} \tag{3-5}$$

Here S_0 is the Coulomb cohesion and ϕ is the Coulomb friction angle. When properly calibrated, fail = 0 indicates the onset of rock failure; fail < 0 denotes catastrophic failure; and fail > 0 predicts stability. Because this model solves for the pressure change brought on by pumping as well as the stresses, strains, and displacements that the pressure change triggers, it calculates the expression just given using the change in pressure than its absolute value.

Results: Failure Criterion

The values for the fail function appear in Figure 3-17. When the fail values become increasingly negative, the potential for failure is higher. As expected, the fail function estimates show the greatest potential for failure just above the split in the well.

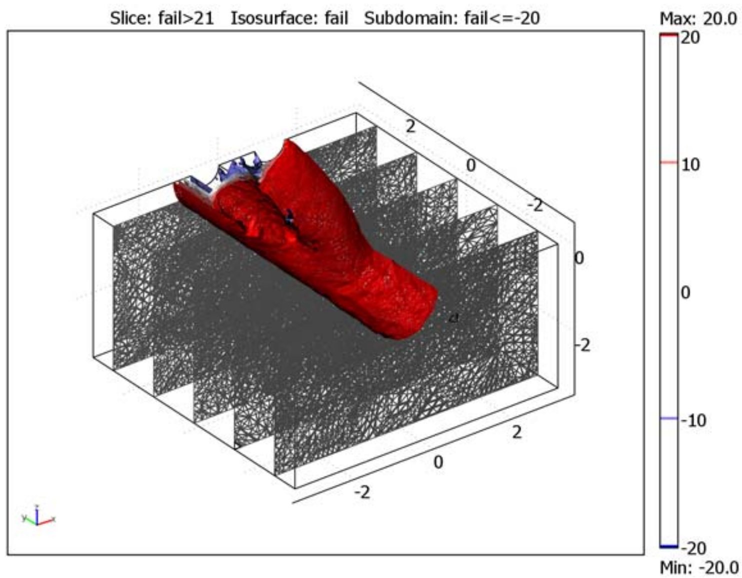


Figure 3-17: Values of the fail function calculated with results from a poroelastic model for the branching junction in an open-hole multilateral well. A negative value for the fail function denotes greater potential for failure.

Conclusions

This example couples fluid flow and solid deformation for a poroelastic analysis using easy-to-use application modes from COMSOL Multiphysics. The analysis provides estimates of the pressure change brought on by pumping as well as the stresses, strains, and displacements that the pressure drop triggers. Combining the simulation results with a 3D Coulomb failure expression, maps vulnerability to mechanical failure from the pumping. The data and geometry for this model come from petroleum industry analyses by TerraTek (Ref. 1), which in turn use failure criteria to map the potential for failure during emplacement of the well in addition to the potential for failure when the well is pumped.

Data

This model uses the coefficients and parameters listed in Table 3-2.

TABLE 3-2: MODEL DATA

VARIABLE	DESCRIPTION	VALUE
ρ_f	Fluid density	0.0361 lb/in^3
κ	Permeability	$1\cdot10^{-13}$ in^2
η	Viscosity	$1\cdot10^{-7}$ psi·s
E	Young's modulus	$0.43\cdot10^6$ psi
ν	Poisson's ratio	0.16
ρ_s	Solids density	0.0861 lb/in^3
p_r	Pressure in reservoir	122.45 psi
p_w	Pressure in well	0 psi
So	Coulomb cohesion	850 psi
ϕ	Coulomb friction angle	31 degrees
C_1	Calibration constant 1	14.7
C_2	Calibration constant 2	40

Reference

1. R. Suarez-Rivera, B.J. Begnaud, and W.J. Martin, "Numerical analysis of open-hole multilateral completions minimizes the risk of costly junction failures," Rio Oil & Gas Expo and Conference (IBP096_04), 2004.

Model Library path: `Earth_Science_Module/Flow_and_Deformation/multilateral_well`

MODEL NAVIGATOR

1 Open the **Model Navigator**.

2 From the **Space dimension** list, choose **3D**.

3 In the list of application modes, select **Earth Science Module>Fluid Flow>Darcy's law>Pressure analysis**. Click the **Multiphysics** button, then click **Add**.

4 In the list of application modes select **COMSOL Multiphysics>Structural Mechanics> Solid, Stress-Strain**. Click **Add**.

5 Click **OK**.

GEOMETRY MODELING

In this example, the geometry already exists in a COMSOL Multiphysics model file.

1 Choose **File>Import>CAD Data From File**.

2 Browse to the folder `Earth_Science_Module>Flow_and_Deformation` in the Model Library root directory.

3 Select the file `multilateral_well.mphbin`, then click **Import**.

The length unit used for the CAD geometry is 1 in. Because COMSOL Multiphysics' default base unit system is SI, with basic length unit 1 m, you need to scale the geometry by the factor 0.0254 along all three coordinate axes to keep the default base unit system. Alternatively, you can change the base unit system to Gravitational IPS, which uses the inch as basic length unit.

As a third option, which is the one exemplified in these modeling instructions, you can scale the geometry by a factor 1/12 and change the base unit system to British engineering units, with basic length unit 1 ft. Thus, complete the geometry-modeling stage with the following steps:

1 Click the **Scale** button on the Draw toolbar.

2 In the **Scale factor** edit fields for **X**, **Y**, and **Z**, type `1/12`. Leave the **Scale base point** at (0, 0, 0).

3 Click **OK**.

4 Click the **Zoom Extents** button on the Main toolbar.

The length unit in the drawing area is now 1 ft.

MODEL SETTINGS

The model data in Table 3-2 is given in pounds and inches. As long as you include the units when entering the data and scale the geometry if required, as just discussed, COMSOL Multiphysics' unit-handling functionality allows you choose whether to use these units also when analyzing the model or change to some other system. Here, to change to British engineering units, proceed as follows:

1 From the **Physics** menu, select **Model Settings**.
2 From the **Base unit system** list, select **British engineering units**.
3 Click **OK**.

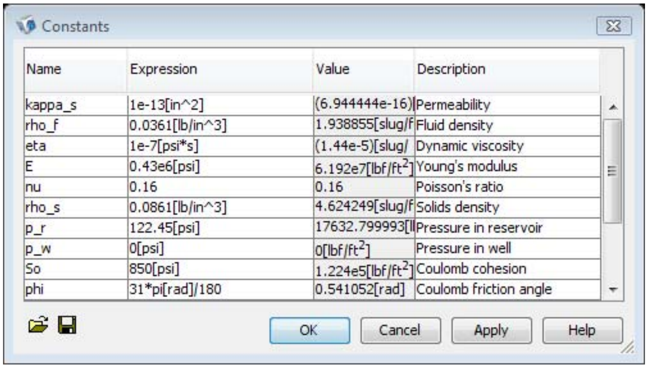
OPTIONS

Constants

Define constants you need in the model or during postprocessing.

1 From the **Options** menu, open the **Constants** dialog box.
2 Enter the following constants in the following table:

NAME	EXPRESSION	DESCRIPTION
kappa_s	1e-13[in^2]	Permeability
rho_f	0.0361[lb/in^3]	Fluid density
eta	1e-7[psi*s]	Dynamic viscosity
E	0.43e6[psi]	Young's modulus
nu	0.16	Poisson's ratio
rho_s	0.0861[lb/in^3]	Solids density
p_r	122.45[psi]	Pressure in reservoir
p_w	0[psi]	Pressure in well
So	850[psi]	Coulomb cohesion
phi	31*pi[rad]/180	Friction angle
C1	14.7	Calibration constant 1
C2	40	Calibration constant 2



3 Click **OK** to close the **Constants** dialog box.

Scalar Expressions

1 From the **Options** menu, choose **Expressions>Scalar Expressions**.

2 Define the following scalar expressions (the descriptions are optional):

NAME	EXPRESSION	DESCRIPTION
`N`	`2*So*cos(phi)/(1-sin(phi))`	`Fail parameter`
`Q`	`(1+sin(phi))/(1-sin(phi))`	`Fail parameter`
`fail`	`(((s3_sld+C1*(p_r-p))-Q*(s1_sld+C1*(p_r-p))+N*(1+(s2_sld-s1_sld)/(s3_sld-s1_sld)))/C2)[1/psi]`	`Fail expression`
`support_x`	`0`	`Well support, x-component`
`support_y`	`0`	`Well support, y-component`
`support_z`	`0`	`Well support, z-component`

Note that the expression fail defined in Equation 3-5 has the dimension of stress. By appending the operator `[1/psi]` to the dimensionful expression enclosed within parentheses you extract its value in psi, which is what Ref. 1 uses. This way, you can analyze the risk for rock failure using the same criteria as in Ref. 1 independently of your choice of base unit system.

3 Click **OK**.

PHYSICS SETTINGS—DARCY'S LAW

Subdomain Settings

1 From the **Multiphysics** menu, select **Darcy's law (esdl)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1.

4 On the **Coefficients** page, select **Permeability** from the drop-down list.

5 Enter the following settings; when done, click **OK**.

QUANTITY	VALUE
κ_s	kappa_s
ρ_f	rho_f
η	eta

6 On the **Init** page, type p_r in the **p(t$_0$)** edit field, then click **OK**.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the following settings; when done, click **OK**.

SETTINGS	BOUNDARIES 1, 3, 13	BOUNDARIES 6–10	BOUNDARIES 2, 4, 5, 11, 12
Boundary condition	Pressure	Pressure	Zero flow/Symmetry
p_0	p_r	p_w	

PHYSICS SETTINGS—SOLID STRESS STRAIN

Subdomain Settings

1 From the **Multiphysics** menu, select **Solid, Stress-Strain (sld)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 On the **Material** page, enter the following settings:

QUANTITY	VALUE/EXPRESSION
E	E
ν	nu
ρ	rho_s

4 On the **Load** page, enter these settings:

QUANTITY	VALUE/EXPRESSION
F_x	-px
F_y	-py
F_z	-pz

5 Click **OK**.

Boundary Conditions

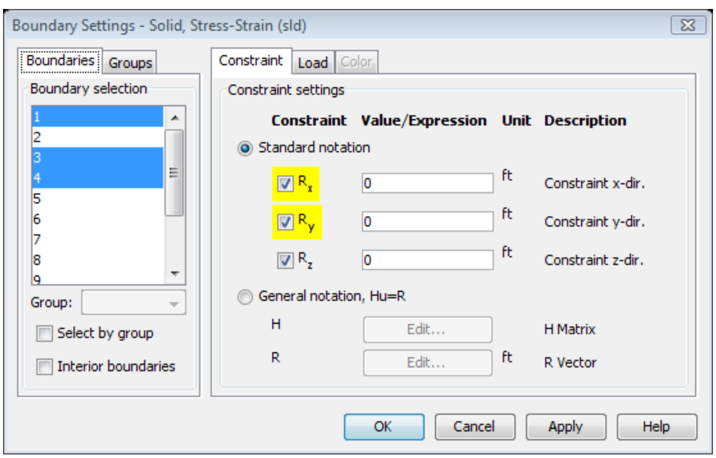
1 From the **Physics** menu, select **Boundary Settings**.

2 On the **Constraints** page, enter these settings:

CONSTRAINT	BOUNDARY	EXPRESSION
R_x	1, 3, 13	0
R_y	1–3, 5, 13	0
R_z	1, 3, 4, 11–13	0

3 On the **Load** page, enter the following settings:

QUANTITY	BOUNDARIES	EXPRESSION
F_x	6–10	`-support_x`
F_y	6–10	`-support_y`
F_z	6–10	`-support_z`



4 Click **OK**.

MESH GENERATION

1 Choose **Mesh>Free Mesh Parameters**.

2 On the **Global** page, select **Coarse** from the **Predefined mesh sizes** list. Click **OK**.

3 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar to start the analysis with the default solver settings.

POSTPROCESSING AND VISUALIZATION

To generate Figure 3-14 on page 186:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, go to the **Plot type** area and select the **Isosurface** and **Streamline** check boxes. Clear the **Slice** check box.

3 Click the **Isosurface** tab. On the **Isosurface Data** page, set the **Expression** to `p` and the **Unit** to `psi`.

4 Click the **Streamline** tab. On the **Streamline Data** page, choose **Darcy's Law (esdl)>Pressure gradient** from the **Predefined quantities** list. On the **Start Points** page, type `60` in the **Number of start points** edit field. On the **Line Color** page, click the **Use expression** button, then click the **Color Expression** button. From the **Predefined quantities** list, choose **Darcy's Law (esdl)>Velocity field**. Clear the **Color scale** check box, then click **OK**. Select **Tube** in the **Line type** list. Click the **Tube Radius** button, then clear the **Auto** check box for **Radius scale factor** and type `0.4` in the associated edit field. Click **OK** to close the **Tube Radius Parameters** dialog box.

5 Click **Apply** to generate the plot.

6 Click the **Headlight** button on the Camera toolbar to add directed light.

To generate Figure 3-15 on page 187:

1 In the **Plot Parameters** dialog box, click the **General** tab.

2 Clear the **Isosurface** and **Streamline** check boxes and select the **Boundary** and **Deformed shape** check boxes in the **Plot type** area.

3 Click the **Boundary** tab.

4 In the **Boundary data** area, select **Solid, Stress-Strain (sld)>Total displacement** from the **Predefined quantities** list. From the **Unit** list, select **in**.

5 Click the **Deform** tab and select **Solid, Stress-Strain (sld)>Displacement** from the **Predefined quantities** list on the **Subdomain Data** page. Click **Apply**.

To generate Figure 3-16 on page 188:

1 Click the **General** tab, then select the **Isosurface** and **Streamline** check boxes in the **Plot type** area. Leave the **Boundary** and **Deformed shape** check boxes unchanged.

2 Click the **Boundary** tab. From the **Fill style** list, select **Wireframe**. Click **Apply**.

3 Click the **Zoom In** button on the Main toolbar.

To generate Figure 3-17 on page 189:

1 Click the **General** tab. In the **Plot type** area, clear the **Streamline**, **Boundary**, and **Deformed shape** check boxes. Select the **Slice** and **Subdomain** check boxes.

2 Click the **Isosurface** tab. On the **Color Data** page, enter `fail` in the **Expression** edit field. Click the **Vector with isolevels** option button and enter `-20:10:20` in the associated edit field. From the **Colormap** list, choose **wave**. With this choice, negative values, zero, and positive values appear in shades of blue, white, and shades of red, respectively.

3 Click the **Subdomain** tab. In the **Color data** area, type `fail<=-20` in the **Expression** edit field. Click the **Range** button. Clear the **Auto** check box. For **min** and **max** enter `0.001` and `1.00`, respectively. Click **OK**. In the **Element color** area, click the **Uniform color** option button, the click the **Color** button. Choose black, then click **OK**.

   This string of steps begins with the expression that assigns fail values less than or equal to –20 with a value of 1 and those greater than –20 with a value of zero. The minimum and maximum data levels serve to cut off values of zero from the plot, so only fail less than or equal to –20 are denoted with a uniform color of black.

4 Finally go to the **Slice** page. In the **Slice data** area, type `fail>21` in the **Expression** edit field. Click the **Range** button. Clear the **Auto** check box. For **min** and **max** enter `0.001` and `1.00`, respectively. Click **OK**. In the **Number of levels** edit fields in the **Slice positioning** area, set the number of **x levels** and **z levels** to `0`, and the number of **y levels** to `5`. In the **Slice color** area, click the **Uniform color** option button, then click **Color**. Choose a gray shade, then click **OK**. Choose **Wireframe** from the **Fill style** list.

5 Click **OK**.

Freezing Soil

Introduction

When wet soil or clay is subjected to freezing temperatures, water in the interstices freezes. Because water expands when it freezes, the surrounding soil deforms. The deformation changes the pressure in the interstices. The combined impacts of the freezing and the deformation affect the water flow.

This model predicts 3-way interactions between stress and strain, fluid flow, and temperature change. This type of analysis is important in assessments related to road and building construction, freeze-thaw weathering, fluid flow, and a number of environmental applications. The model that follows comes from a COMSOL client who used the results to assess thermo-mechanical impacts in a transportation study.

This analysis couples equations that predict what happens when a water-filled soil core freezes from the center outwards. Included in the analysis are:

- Effects of a stepwise change in the thermomechanical properties at the phase transition temperature
- Porous fluid-flow behavior involving a temperature-driven contribution
- Stress-strain behavior including loads from thermal expansion and fluid flow
- Heat conduction including phase change and the latent heat of freezing
- Coupling effects between the above-mentioned phenomena.

This discussion assumes temperature changes are fully transient with a quasi-static interaction with fluid flow and solid deformation. The model uses the Darcy's Law and the Convection and Conduction application modes from the Earth Science Module. It also employs a Stress-Strain application mode from the Structural Mechanics Module, an application mode that automates temperature-deformation coupling.

Model Definition[1]

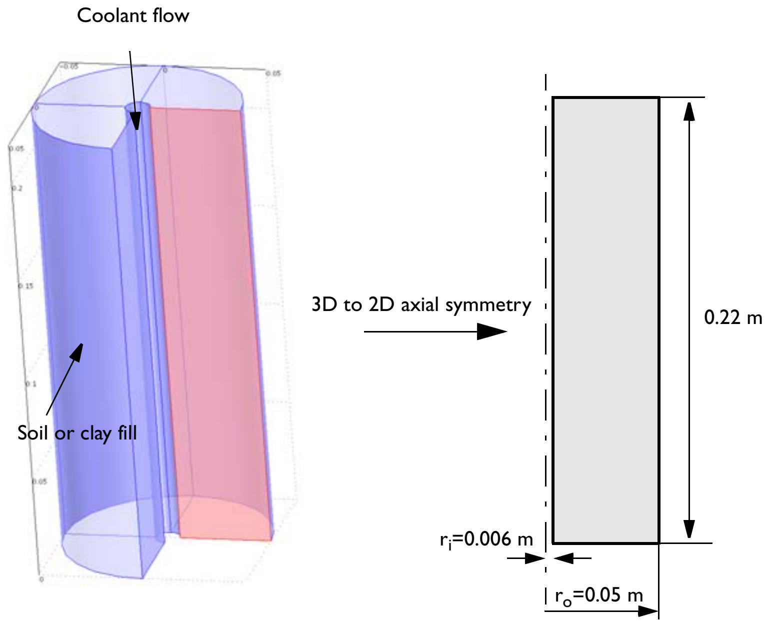


Figure 3-18: Experimental setup for investigations of freezing soil. A symmetry observation permits modeling in axisymmetry 2D.

The model geometry is based on a general test rig often used for investigating the properties of soil and clay (see Figure 3-18). A cylindrical container with the sample soil has a concentric channel, through which a coolant fluid flows. The initial temperature of the wet soil is +3 °C. As the coolant at −15 °C enters the pipe, a freezing front travels outward in the soil specimen. Because the soil is homogeneous, you can take advantage of the geometric symmetry and model the phenomena in 2D.

STRESS-STRAIN EQUATIONS

The fundamental Navier's equation describes a force equilibrium

$$-\nabla \cdot \sigma = \mathbf{F} \tag{3-6}$$

where σ is the stress tensor and $\mathbf{F}$ is a volume force.

The entries of the stress tensor for axisymmetry are

1. Model definition and material data courtesy of Dr. J.P.B.N. Derks, Ministry of Transport, Public Work & Water Management, the Netherlands.

$$\sigma = \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{xy} \\ \tau_{xz} \\ \tau_{yz} \end{bmatrix}$$

where τ denotes off-diagonal components of strain or shear.

The equations simplify to two force balances in the r and z directions:

$$\frac{\partial \sigma_r}{\partial r} + \frac{\partial \tau_r}{\partial r} + \frac{\sigma_r - \sigma_\theta}{r} + F_r = 0 \tag{3-7}$$

$$\frac{\partial \tau_{rz}}{\partial r} + \frac{\partial \sigma_z}{\partial r} + \frac{\tau_{rz}}{r} + F_z = 0 \tag{3-8}$$

where τ denotes off-diagonal components of strain or shear.

Flow-to-Structure Coupling

When considering the impacts of fluid flow on structural deformation, the stress tensor decompose into two parts

$$\sigma = \sigma' + \mathbf{m}p \tag{3-9}$$

where σ is the total stress, σ' is the so-called grain stress, and p is the pressure of the fluid moving through a porous sand or clay matrix.

In this analysis

$$\mathbf{m} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}^T .$$

Temperature-to-Structure Coupling

The thermomechanical relationship is given by the generalized Hooke's law for an elastic nonisothermal material as in

$$\sigma' = \mathbf{D}(\varepsilon - \varepsilon_{th}) , \qquad \varepsilon_{th} = \alpha(T - T_{ref}) . \tag{3-10}$$

Here $\mathbf{D}$ is the elasticity matrix, σ' represents the elastic stress, ε gives the total strain, and ε_{th} is the thermal strain. Further, α (K^{-1}) is the coefficient of thermal expansion, T is the temperature, and T_{ref} is the strain reference temperature.

FLUID FLOW EQUATIONS

Model the flow with the modified Darcy's law

$$\mathbf{u} = -\frac{\kappa}{\eta}\nabla(p+\phi_s) \tag{3-11}$$

where $\mathbf{u} = (u, v, w)$ denotes the vector of fluid velocities in the x, y, and z directions, and ϕ_s is the suction pressure.

Temperature-to-Flow Coupling, Segregation Potential

The fluid flow and temperature relationships couple through the term

$$\phi_s = SP_0 \cdot T/\kappa,$$

where SP_0 is the *segregation potential* (kg·m/(s^2·K)), which is the ratio of the moisture migration velocity to the temperature gradient in a freezing soil, and κ is the permeability (m^2). The segregation potential SP_0 is a positive constant below the freezing point and 0 above. Experimental observations on specimens frozen under a temperature gradient suggest that, even though much of the pore water is frozen, water transport still occurs in the frozen soil past the pore freezing front in response to temperature-induced unfrozen water content gradients and suction gradients in these unfrozen water films. The migratory water freezes at the segregation freezing temperature, T_s, which is lower than the pore freezing temperature T_p (Ref. 1). In this model example, it is assumed that the segregation freezing temperature is well below the temperature range of the study.

Given the definition for ϕ_s, Equation 3-11 states that the fluid velocities depend on the pressure gradient and the temperature gradient for conditions below the freezing point.

Structure-to-Flow Coupling

For quasi-steady flow, the following relationship holds:

$$\nabla \cdot \mathbf{u} = -(\dot{\varepsilon}_{xx} + \dot{\varepsilon}_{yy} + \dot{\varepsilon}_{zz}), \tag{3-12}$$

where $\dot{\varepsilon}_{xx}$ and similar terms are the *rates of strain* (s^{-1}) from the stress-strain equations.

Combining Equation 3-11 and Equation 3-12 gives the governing equation

$$\nabla \cdot \left(-\frac{k}{\eta}\nabla(p+\phi_s)\right) = -(\dot{\varepsilon}_{xx} + \dot{\varepsilon}_{yy} + \dot{\varepsilon}_{zz}), \tag{3-13}$$

which this example models with the Darcy's Law application mode.

TEMPERATURE EQUATIONS

This problem uses the well-known heat equation to model the transfer of heat. As described in the *Earth Science Module User's Guide*, the heat transfer equation reads

$$\rho c_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q .$$

Results

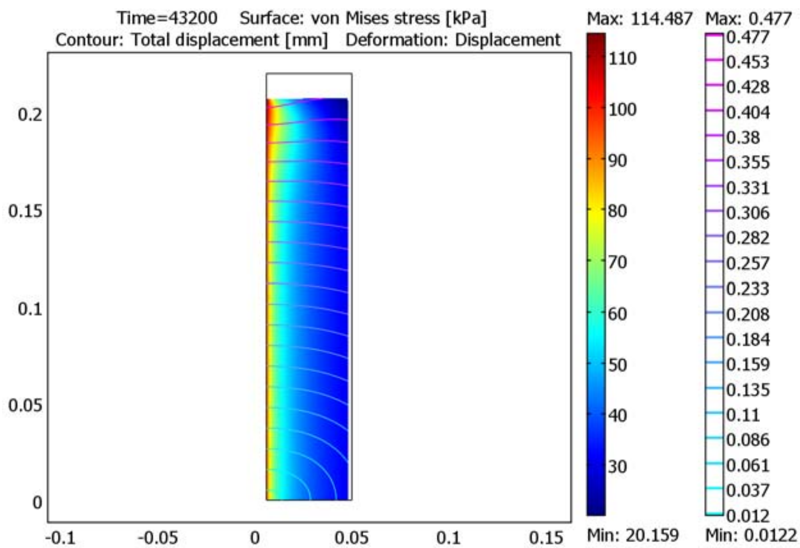


Figure 3-19: A snapshot of the von Mises stresses (surface plot) and displacements (contours) in a column of freezing soil.

Figure 3-19 shows the displacements in the solid sample and the von Mises stresses after 12 hours of freezing operation. It is also easy to monitor how the physical properties of the sand change with time and space; see Figure 3-20.

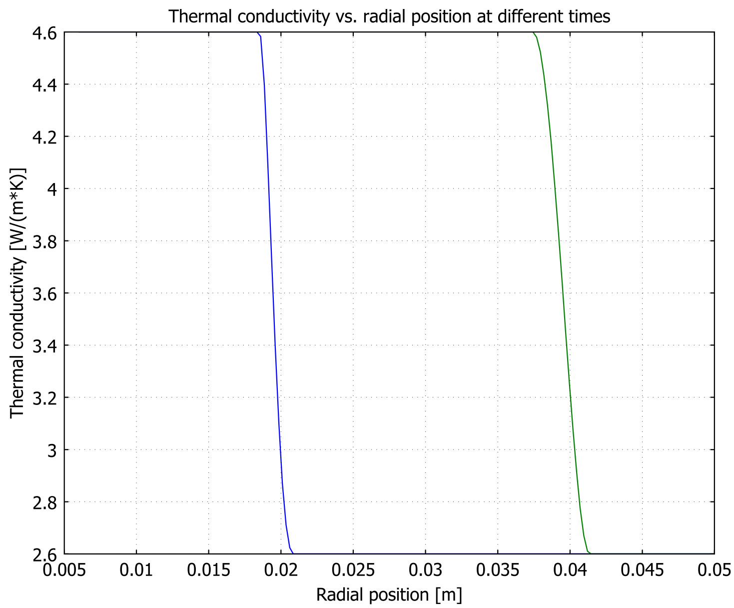


Figure 3-20: Thermal conductivity changes in a step at the freezing point. The lower curve corresponds to 24 minutes, and the upper curve to 7 hours and 12 minutes.

Reference

1. Jean-Marie Konrad, "Estimation of the segregation potential of fine-grained soils using the frost heave response of two reference soils," *Can. Geotech. J.*, vol. 42, pp. 38–50, 2005.

Modeling in COMSOL Multiphysics

Turning to the COMSOL Multiphysics Structural Mechanics Module, you choose the Axial Symmetry, Stress-Strain application mode to solve Equation 3-7 and Equation 3-8. To account for the fluid pressure according to Equation 3-9, simply add

$$\begin{bmatrix} -\frac{\partial p}{\partial r} \\ -\frac{\partial p}{\partial z} \end{bmatrix}$$

to the body load vector $\mathbf{F}$ on the **Load** page in the **Subdomain Settings** dialog box. To have that application mode automatically account for the thermomechanical relations, Equation 3-10, select the **Include thermal expansion** check box on the **Load** page. To get easy access to the rates of strain (time derivatives of the strain), use a time-dependent stress-strain analysis. This solves Equation 3-6 with an extra term on the left-hand side, namely $\rho(\partial^2\mathbf{u})/(\partial t^2)$, which is the acceleration term in Newton's second law. Here, $\mathbf{u}$ is the vector of directional deformations (in m). However, you can make the assumption that the time scale in the mechanical problem is much shorter than that for the heat transfer problem. Here you skip the time-derivative term in the stress/strain equation by setting $\rho = 0$ and still access the rates of strain as described in the next paragraph.

It is easy to implement the modified Darcy's law (Equation 3-8) with the Earth Science Module's Darcy's Law application mode, and its predefined equation is

$$\nabla \cdot \left(-\frac{\kappa}{\eta}\nabla(p + \rho_f g D)\right) = Q_s . \tag{3-14}$$

Because the vertical change is small, you can ignore gravity impacts on flow. There is, however, another contribution to the mass flux, namely that from the segregation potential (see Equation 3-13). Include this contribution by setting $D = \phi_s/(g\rho_f)$.

Next place the rate-of-strain expression in Equation 3-12 in the Q_s term. The r, ϕ, and z components of the rate of strain, $\dot{\varepsilon}_{rr}$, $\dot{\varepsilon}_{\phi\phi}$ and $\dot{\varepsilon}_{zz}$, are readily available in the time-dependent Axial Symmetry, Stress-Strain application mode as the expressions `diff(er_stress,t)`, `diff(ephi_stress,t)`, and `diff(ez_stress,t)`. Hence, enter `-(diff(er_stress,t)+diff(ephi_stress,t)+diff(ez_stress,t))` in the Q_s edit field of the Darcy's Law application mode.

The model handles the stepwise-changing material properties at the freezing point as well as the latent heat of freezing as described in "Phase Change" on page 303 in the *Earth Science Module Model Library.*

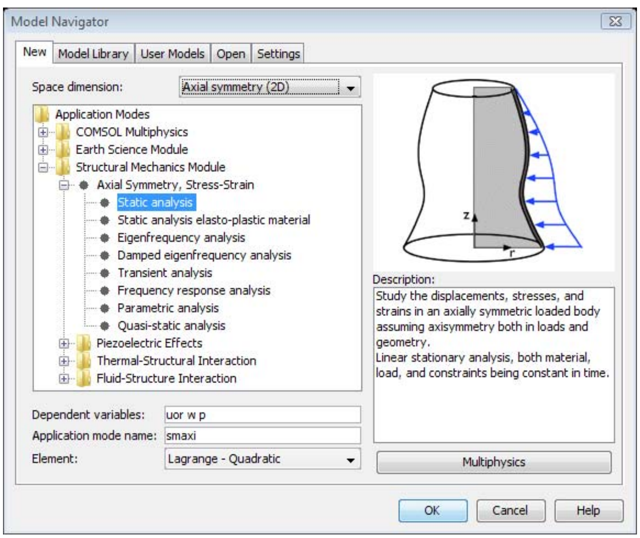
Note: This model requires the Earth Science Module and the Structural Mechanics Module.

Model Library path: `Earth_Science_Module/Flow_and_Deformation/freezing_soil`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 In the **Model Navigator**, select **Axial symmetry (2D)** from the **Space dimension** list and then in the list of application modes select **Structural Mechanics Module>Axial Symmetry, Stress-Strain>Static analysis**. In the **Application mode name** edit field, type `stress`.



2 Click the **Multiphysics** button, then click **Add**.

3 Return to the list of application modes and select **COMSOL Multiphysics> Heat Transfer>Conduction>Transient Analysis**. In the **Application mode name** edit field enter `heat`, then click **Add**.

4 In the list of application modes select **Earth Science Module>Fluid Flow>Darcy's Law>Pressure analysis**. In the **Application mode name** edit field enter `Darcy`, then click **Add**.
5 Click **OK**.

OPTIONS

1 From the **Options** menu select **Constants** and enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
T_trans	0[degC]	Freezing point
scale	0.5	Width of smoothed step function
rho_sa	2000[kg/m^3]	Density
nu0	0.3	Poisson's ratio
alpha_s	0.8e-6[1/K]	Coefficient of thermal expansion
T_init	3[degC]	Intial temperature
k_sf	4.6[W/(m*K)]	Thermal conductivity below freezing point
k_s	2.6[W/(m*K)]	Thermal conductivity above freezing point
Cp_sf	1000[J/(kg*K)]	Heat capacity below freezing point
Cp_s	1350[J/(kg*K)]	Heat capacity above freezing point
kappa_s	7.1e-5[m^2]	Permeability, unfrozen sand
eta_s	0.001[Pa*s]	Dynamic viscosity
E0_s	65[MPa]	Young's modulus
t_load	300[kN/m^2]	Top edge load
e_load	300[kN/m^2]	Side edge load
dT	0.5[K]	Half width of Gauss bell curve
lam	333[kJ/kg]	Latent heat of freezing
p_pore	150[kPa]	Pore pressure

GEOMETRY MODELING

1 Shift-click the **Rectangle/Square** button at the top of the Draw toolbar.
2 In the **Size** area, set the **Width** to `0.044` and the **Height** to `0.22`.
3 In the **Position** area, select **Center** from the **Base** list. Set **r** to `0.028` and **z** to `0.11`.
4 Click **OK**, then click the **Zoom Extents** button on the Main toolbar.

EXPRESSION DEFINITIONS

From the **Options** menu select **Expressions>Scalar Expressions**, then add the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
HS	flc1hs((T-T_trans)[1/K],scale)	Smoothed Heaviside step
k_g	k_sf+(k_s-k_sf)*HS	Varying thermal conductivity
D	exp(-(T-T_trans)^2/dT^2)/ sqrt(pi*dT^2)	Smoothed Dirac delta function
Cp	Cp_sf+(Cp_s-Cp_sf)*HS	Varying heat capacity
T_b	T_init+18[K]*(1- 2*flc1hs(t[1/s],100))	Varying boundary temperature
Sp0	(1-HS)*1e-12[kg*m/(s^2*K)]	Varying segregation potential

The unit brackets `[1/K]` and `[1/s]` make the function inputs dimensionless.

PHYSICS SETTINGS

Application Scalar Variables

To include the segregation potential mass-flux term in the way described below Equation 3-14, you need to modify the application scalar variable D_{Darcy}.

1 From the **Physics** menu, select **Scalar Variables**.

2 In the **Expression** column for **D_Darcy**, type `(Sp0*T/kappa_s)/ (g_Darcy*rhof_Darcy)`.

3 Click **OK** to close the **Application Scalar Variables** dialog box.

Subdomain Settings—Axial Symmetry, Stress-Strain

1 From the **Multiphysics** menu, select **Axial Symmetry, Stress-Strain (stress)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1, then enter the values in the following table:

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
E	E0_s	Young's modulus
ν	nu0	Poisson's ratio
α	alpha_s	Thermal expansion coeff.

4 On the **Load** page, select the **Include thermal expansion** check box.

5 Specify the loads as in the following table; when done, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
F_r	`-p2r`	Body load (force/volume) r dir.
F_z	`-p2z`	Body load (force/volume) z dir.
Temp	`T`	Strain temperature
Tempref	`T_init`	Strain ref. temperature

Boundary Conditions—Axial Symmetry, Stress-Strain

1 Select the menu **Physics>Boundary Settings**.

2 On the **Constraint** page select Boundaries 1 and 2. From the **Constraint condition** list select **Roller**.

3 Click the **Load** tab. Select Boundary 3, and set $\mathbf{F_r}$ to `0` and $\mathbf{F_z}$ to `-t_load`.

4 Select Boundary 4. Set $\mathbf{F_r}$ to `-e_load` and $\mathbf{F_z}$ to `0`.

5 Click **OK**.

Subdomain Settings—Heat Transfer

1 From the **Multiphysics** menu select **Heat Transfer by Conduction (heat)**.

2 Choose **Physics>Subdomain Settings**, then specify these settings:

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
k (isotropic)	`k_g`	Thermal conductivity
ρ	`rho_s`	Density
C_p	`Cp+D*lam`	Heat capacity

3 On the **Init** page, set $\mathbf{T(t_0)}$ to `T_init`. Click **OK**.

Boundary Conditions—Heat Transfer

1 Choose **Physics>Boundary Settings** and select Boundary 1. From the **Boundary condition** list select **Temperature**, then in the **Temperature** edit field type `T_b`.

2 Select Boundary 4. In the **Boundary condition** list select **Temperature**, then in the **Temperature** edit field type `T_init`. Click **OK**.

Subdomain Settings—Darcy's Law

1 Select the menu item **Multiphysics>Darcy's Law (Darcy)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Specify the following settings; when done, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
κ_s	`kappa_s`	Saturated permeability
ρ_f	`1`	Density, liquid
η	`eta_s`	Viscosity, liquid
Q_s	`-(diff(er_stress,t)+diff(ephi_stress,t) +diff(ez_stress,t))`	Liquid source

Because of the setting for D on page 207, the density value has to be nonzero but is otherwise irrelevant.

Boundary Conditions—Darcy's Law

Choose **Physics>Boundary Settings**, then select Boundary 1. In the **Boundary condition** list select **Pressure**, then set $\mathbf{p_0}$ to `p_pore`. Similarly select Boundary 4 and set the **Pressure** to `0`. Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 Click the **Boundary** tab and select Boundary 1. In the **Maximum element size** edit field enter `0.003`.

3 Click **Remesh**. When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 In the **Times** edit field, type `0:1440:43200`. This provides 30 equidistant time steps during a total simulation time of 12 hours (43,200 s).

3 In the **Absolute tolerance** edit field, type `uor 1e-6 w 1e-6 T 0.001 p2 10`. This sets up absolute tolerances of 10^{-6} for the displacement variables, 0.001 for the temperature, and 10 for the pressure. Click **OK**.

4 Click the **Solve** button on the Main toolbar to compute the solution.

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 3-19, follow these steps.

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, go to the **Plot type** area and select the **Surface**, **Contour**, **Deformed shape**, and **Geometry edges** check boxes.

3 Click the **Surface** tab, then in the **Predefined quantities** list on the **Surface Data** page select **Axial Symmetry, Stress-Strain (stress)>von Mises Stress**.
4 From the **Unit** list, select **kPa**.
5 Click the **Contour** tab, and in the **Predefined quantities** list on the **Contour Data** page select **Axial Symmetry, Stress-Strain (stress)>Total displacement**.
6 From the **Unit** list, select **mm**.
7 Click **OK** to close the **Plot Parameters** dialog box and generate the plot.

4

Solute Transport Models

In this chapter you find models of solute transport, including solute injection, variably saturated flow, and pesticide transport and reaction.

Solute Injection

Introduction

Predicting the transport of contaminants that move with subsurface fluids generally means analyzing at least two physics. This model tracks a contaminant that enters an aquifer at a point, such as an injection well or toxic spill, and spreads through the aquifer with time. The model has an analytic solution developed by Wilson and Miller (Ref. 1), which has been used to test several dedicated fluid flow and transport codes. The particular problem in this model comes from the MT3DMS manual of Zheng and Wang (Ref. 2).

The analysis models steady-state fluid flow and follows up with a transient solute-transport simulation; it employs the Darcy's Law application mode and the Solute Transport application mode from the Earth Science Module. In COMSOL Multiphysics it is straightforward to specify a fluid velocity without solving a flow problem. This example solves for the velocities to demonstrate the mechanics of coupling flow and transport simulations in one model file.

The example also shows how to use the solver settings for the combined steady-state and transient solution. The instructions detail how to model a point source using the point flux settings available in the Earth Science Module.

The first section in this discussion gives an overview of the problem. Next it gives the equations and describes how the fluid flow and the solute transport application modes link in COMSOL Multiphysics. Next come a few implementation details including a table of model data. The results shown next then illustrate various postprocessing options. The last section describes how to build the model using the COMSOL Multiphysics graphical user interface.

Model Definition

In this example, there is regional flow from left to right across a 450 m × 300 m aquifer. The fluid moves at a Darcy velocity of 0.11 m/d. The aquifer has homogeneous and isotropic material properties. A point source releases a small amount of fluid into the aquifer at 1 m^3/d, a release rate small enough that the flow field remains uniform. The injected fluid carries a nonreactive solute at a concentration of 1000 ppm. The contaminant migrates by advection and dispersion and never reaches a boundary. The aquifer is initially pristine with concentrations everywhere equal to zero. The only source of contaminant is the injection, so flow through the inlet has zero concentration. The period of interest is one year.

FLUID FLOW

Darcy's law describes the fluid flow in this problem. With the hydraulic-head formulation, the governing equation is

$$\nabla \cdot [-K\nabla H] = Q_s$$

where K is hydraulic conductivity (m/d), H is hydraulic head (m), and Q_s is the volume flow rate of fluid per unit volume of aquifer (d^{-1}).

The point source is

$$Q_s = \frac{W}{b}\delta(x - x_i, y - y_i)$$

where W is the volumetric pumping rate W (m^3/d); b is the aquifer thickness; δ denotes the Dirac delta function, which is nonzero only in the point (x_i, y_i), where x_i and y_i are the well coordinates.

Because the flow field is at steady state, you can obtain a unique solution by specifying the model geometry, the point source, the material properties, and the boundary conditions. The problem statement gives the hydraulic head at the inlet and the outlet and indicates symmetry conditions on the sides. In the Darcy's Law application mode, you express these boundary conditions as

$$\begin{array}{ll} \mathbf{n} \cdot [K\nabla H] = 0 & \partial\Omega \ \text{Sides} \\ H = H_{\text{in}} & \partial\Omega \ \text{Inlet} \\ H = 0 & \partial\Omega \ \text{Outlet} \end{array}$$

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

COUPLING

The groundwater-flow and solute-transport equations given here are linked by the Darcy velocity, $\mathbf{u} = -K\nabla H$, which gives the specific flux (m/d) of fluid across an infinitesimal surface representing both the solids and the pore spaces. COMSOL Multiphysics computes the Darcy velocity vector $\mathbf{u}$, which consists of the x and y directional velocities denoted u and v, respectively.

SOLUTE TRANSPORT

The advection-dispersion equation governs solute transport in this problem:

$$\theta_s \frac{\partial c}{\partial t} + \nabla \cdot [-\theta_s D_L \nabla c + \mathbf{u} c] = S_c$$

Here D_L is the hydrodynamic dispersion tensor (m^2/d); θ_s denotes the fluid volume fraction; c gives the dissolved concentration (kg/m^3); $\mathbf{u}$ is the Darcy velocity (m/d); and S_c represents the quantity of solute added per unit volume of porous medium per unit time ($\mathrm{kg}/(\mathrm{m}^3 \cdot \mathrm{d})$).

The entries for the dispersion tensor are

$$\theta D_{Lii} = \alpha_1 \frac{u_i^2}{|\mathbf{u}|} + \alpha_2 \frac{u_j^2}{|\mathbf{u}|}$$

$$\theta D_{Lij} = \theta D_{Lji} = (\alpha_1 - \alpha_2) \frac{u_i u_j}{|\mathbf{u}|}$$

where D_{Lii} are the principal components of the dispersion tensor; D_{Lji} and D_{Lji} are the cross terms; α represents the dispersivity (m); and the subscripts "1" and "2" denote longitudinal and transverse flow, respectively.

In this problem, S_c represents the solute injected at the point well, which is defined by

$$S_c = Q_s c_Q = \frac{W}{b} c_Q \delta(x - x_i, y - y_i)$$

where c_Q is the concentration of the solute in the water (kg/m^3). You implement the solute injection with the same logic as the fluid point source.

The problem statement specifies that the only contaminant source in the aquifer is the point well, and the boundaries are far enough from the injection well that the contaminant never leaves the model domain. You thus set the inlet concentration to zero and assign the other boundaries an advective flux. The expressions for these boundary conditions are

$$\begin{array}{ll} \mathbf{n} \cdot [-\theta_s D_L \nabla c] = 0 & \partial\Omega \text{ Sides} \\ c = 0 & \partial\Omega \text{ Inlet} \\ \mathbf{n} \cdot [-\theta_s D_L \nabla c] = 0 & \partial\Omega \text{ Outlet} \end{array}$$

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

Data

Build the model with the following data:

PARAMETER	NAME	VALUE
K	Hydraulic conductivity	1 m/d
ρ_f	Fluid density	1000 kg/m^3
g	Gravity	9.82 m/s^2
u	Darcy velocity	0.11 m/d
W	Pumping rate	1 m^3/d
b	Aquifer thickness	10 m
H_{in}	Inlet head	45 m
θ_s	Porosity	0.3
α_1	Longitudinal dispersivity	10 m
α_2	Transverse horizontal dispersivity	3 m
c_s	Solute concentration at source	1000 ppm

Results

Figure 4-1 shows the solution to the steady-state flow problem. The hydraulic head drops from the inlet to the outlet, and the velocity field is almost uniform, as required in the problem statement (Ref. 1).

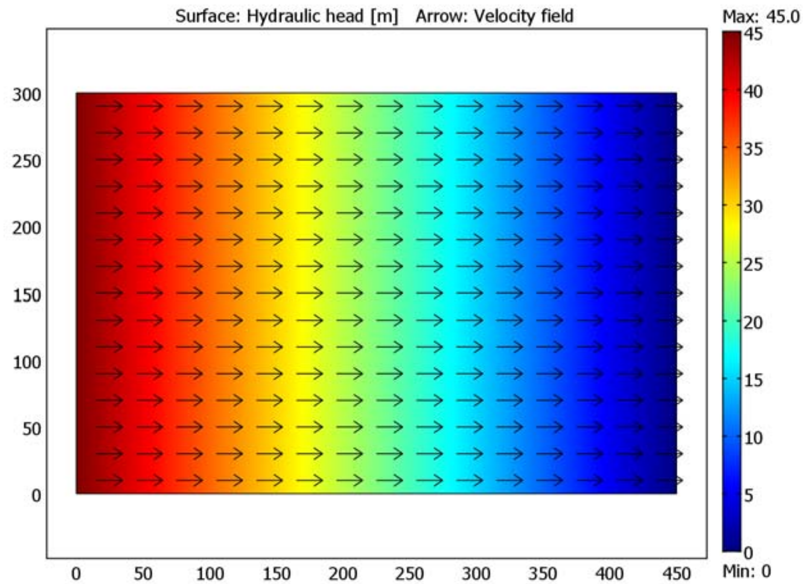


Figure 4-1: COMSOL Multiphysics solution of almost uniform Darcy flow in a domain with a small point leak. Shown are the hydraulic head (surface plot) and velocity field (arrows).

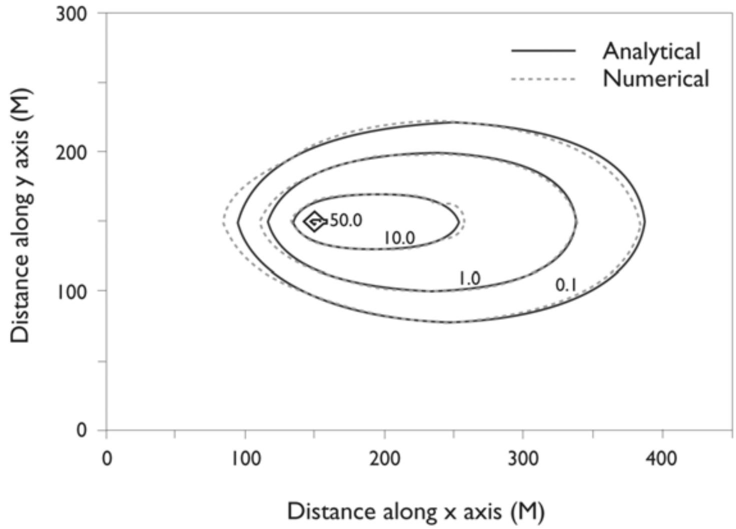


Figure 4-2: COMSOL Multiphysics results for the solute-transport problem are a near perfect match to the analytic solution of Ref. 1, which is shown with the numerical estimates of Ref. 2.

Figure 4-3 illustrates the evolution of the contaminant plume with snapshots at 30 days, 100 days, and 360 days. The solute plume spreads in time but never reaches the boundary. In creating these plots, the author clipped off concentrations below 0.1 ppm and used an expression containing logical operators to give the same shading to zones with concentrations of 50 ppm or greater.

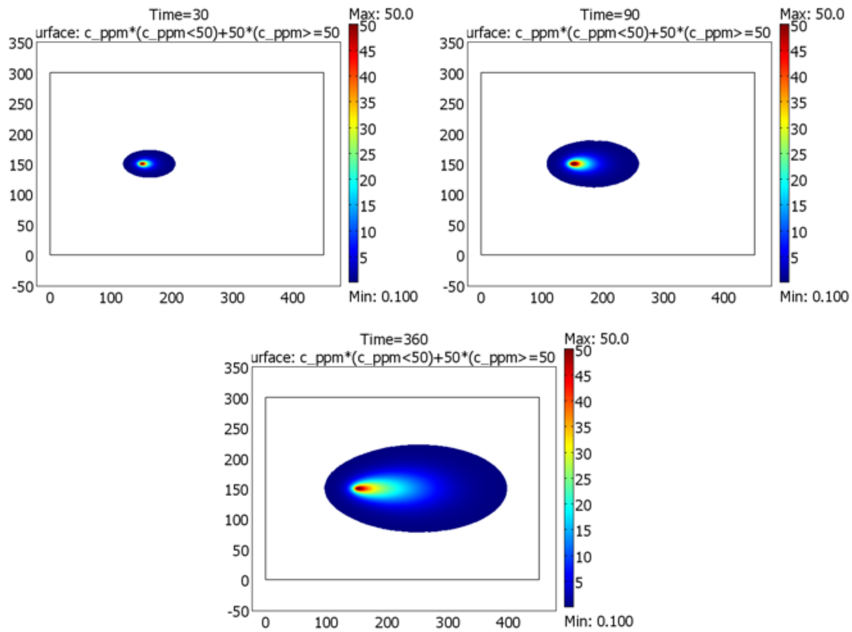


Figure 4-3: Concentrations at 30 days (top left), 100 days (top right), and 360 days (bottom) for 2D fluid flow and solute transport for a continuously injecting point source; shown are concentrations from 0.1 ppm to 50 ppm or greater.

In the user interface you can interactively view the value at a given point by either clicking at the point of interest or entering the point coordinates to trigger a numeric readout. You can also obtain numeric results for the arbitrary expressions along a line or within a subdomain using cross-section and domain plots. The cross sections in Figure 4-4 and Figure 4-5, for example, illustrate the dispersive and advective components of the solute flux. The flux from chemical diffusion is zero. The COMSOL Multiphysics solution shown here gives results along the line y = 150 m at 10, 30, 90, 180, and 360 days.

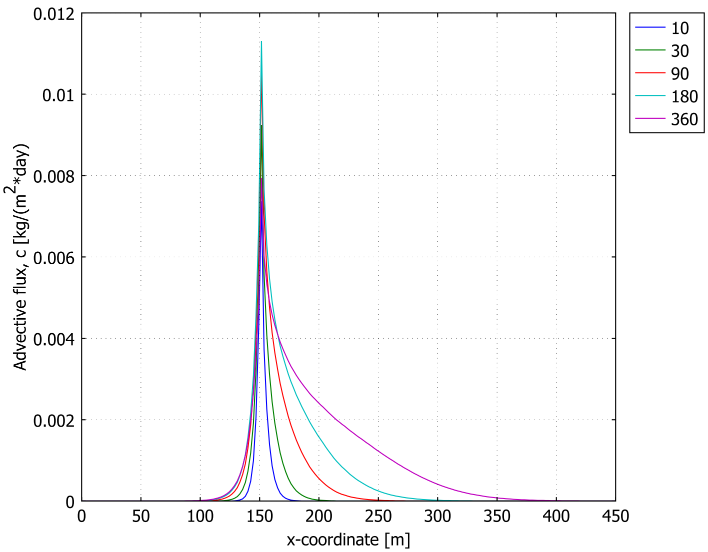


Figure 4-4: Advective flux along y = 150 m at 10, 30, 90, 180, and 360 days.

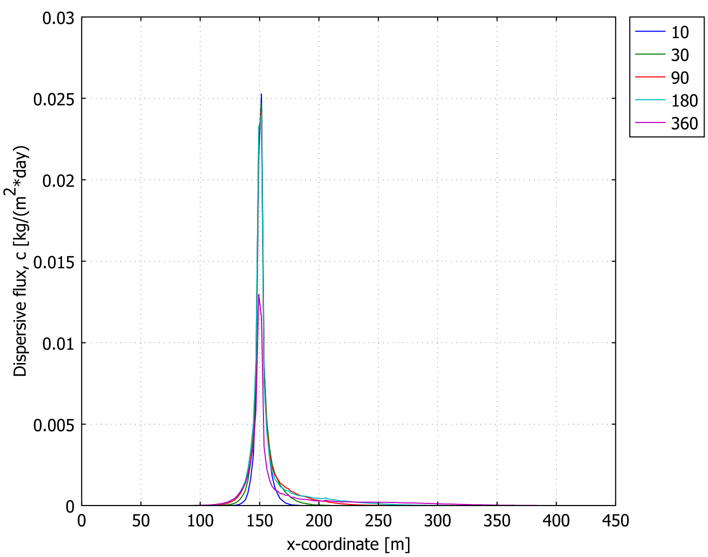


Figure 4-5: Dispersive flux along y = 150 m at 10, 30, 90, 180, and 360 days.

Figure 4-6 gives the solute concentration as a combined color and height plot.

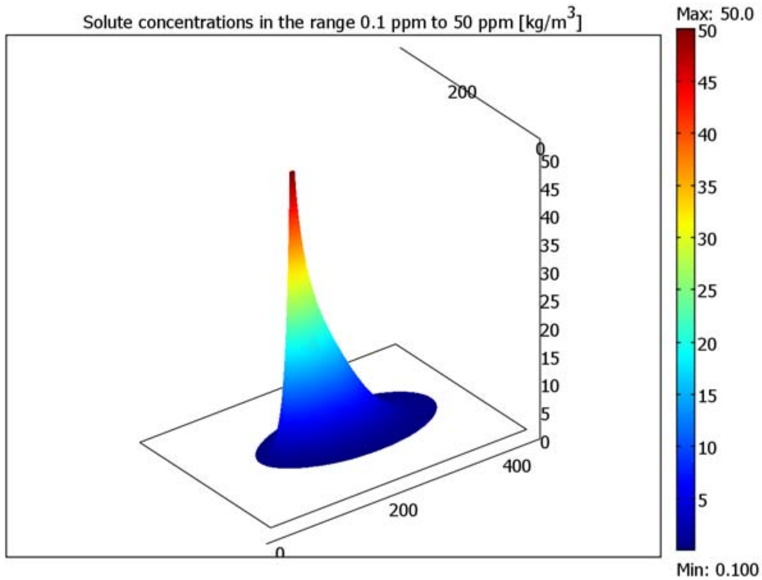


Figure 4-6: Solute concentrations from 0.1 ppm to 50 ppm at 360 days.

References

1. J.L. Wilson and P.J. Miller, "2D plume in uniform ground-water flow," *J. Hyd. Div., ASCE*, vol. 4, pp. 503–514, 1978.

2. C. Zheng and P. Wang, *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems*, University of Alabama, 1998.

Model Library path: `Earth_Science_Module/Solute_Transport/solute_injection`

Modeling Using the Graphical User Interface

The first step is to open COMSOL Multiphysics and set up two application modes.

MODEL NAVIGATOR

1 Open the **Model Navigator**, and from the **Space dimension** list select **2D**.
2 From the list of application modes choose **Earth Science Module>Fluid Flow>Darcy's Law>Hydraulic head analysis**.
3 Click the **Multiphysics** button, then click **Add**.
4 From the list of application modes choose **Earth Science Module>Solute Transport>Saturated Porous Media>Transient analysis**.
5 Click **Add**, then click **OK**.

GEOMETRY MODELING

1 Go to the **Draw** menu and select **Specify Objects>Rectangle**.
2 Specify a width of 450 and height of 300. Click **OK**.
3 Click the **Zoom Extents** button on the Main toolbar to center the rectangle in the field of view.
4 Choose the menu item **Draw>Specify Objects>Point**. In both the **x** and **y** edit fields enter 150. Click **OK**.

OPTIONS AND SETTINGS

Constants

1 From the **Options** menu, select **Constants**.
2 Enter the following names, expressions, and descriptions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
W	1[m^3/s]	Pumping rate
b	10[m]	Aquifer thickness
H_in	45[m]	Inlet head
rho_f	1000[kg/m^3]	Fluid density
c_s	1[kg/m^3]	Solute concentration at source
SPD	1[day/s]	Seconds per day

Scalar Expressions

1 From the **Options** menu, select **Scalar Expressions**.

2 Define the following expression for the solute concentration expressed in parts per million:

NAME	EXPRESSION	DESCRIPTION
`c_ppm`	`1e6*c/rho_f`	`Solute concentration in ppm`

3 Click **OK**.

APPLICATION SCALAR VARIABLES

In the Darcy's Law application mode (**esdl**), the vertical dimension **D_esdl** is the y-axis on your screen and the gravitational acceleration is **g_esdl** is 9.82 $\mathrm{m/s^2}$. Because this model describes a horizontal plane and the time unit is 1 day, you need to modify the value of **g_esdl**.

1 From the **Physics** menu, choose **Scalar Variables**.

2 Make the following changes; when done, click **OK**.

NAME	EXPRESSION
D_esdl	`0`
g_esdl	`9.82[m/s^2]*SPD^2`

With this change of **g_edsl**, the effective time unit in the model becomes 1 day. Thus, wherever the user interface displays the time unit 1 s, read 1 day instead. This also applies in postprocessing, so you must multiply any quantity containing the dimension time to some power n by SPD^n for the units displayed in the user interface and in plots to be correct. For example, when plotting the pressure, p, use the expression `p/SPD^2`, because pressure scales with time, T, as T^{-2}.

PHYSICS SETTINGS—DARCY'S LAW

To set up the steady-state flow model you activate the Darcy's Law application mode, enter material properties for the subdomain, give the boundary conditions, and then set the point flux.

Subdomain Settings

1 From the **Multiphysics** menu, select **Darcy's Law (esdl)**.

2 From the **Physics** menu select **Subdomain Settings**.

3 Verify that the model defaults are the coefficient values you need; when done, click **OK**.

PROPERTY	VALUE
K_s	1
ρ_f	1000

Boundary Conditions

From the **Physics** menu select **Boundary Settings**, then enter the following data; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2, 3	BOUNDARY 4
Boundary condition	Hydraulic head	Zero flux/ Symmetry	Hydraulic head
H_0	`H_in`		0

Point Settings

1 From the **Physics** menu select **Point Settings**.

2 On the **Flux** page, select Point 3.

3 Iin the $\mathbf{N_0}$ edit field for the flux, type `W/b`.

4 Click **OK**.

PHYSICS—SOLUTE TRANSPORT

To set up the transient solute-transport model, you activate the corresponding application mode, enter material and solute properties for the subdomain, specify boundary conditions, and finish with the point flux.

Subdomain Settings

1 From the **Multiphysics** menu, select **Solute Transport (esst)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 On the **Flow and Media** page specify information about the flow field and velocities from the **Darcy's Law (esdl)** application mode.

PARAMETER	EXPRESSION
θ_s	`0.3`
u	`u_esdl`
v	`v_esdl`

Unless you specify otherwise, COMSOL Multiphysics denotes the x- and y-velocities as u and v. Because velocities are not dependent variables in the Darcy's Law application mode, they are application mode variables that COMSOL Multiphysics evaluates using information from the solution. The software denotes application mode variables according to application mode name; here it is **u_esdl** for the x-velocity and **v_esdl** for the y-velocity.

4 On the **Liquid** page, set the dispersivities that describe spreading for solutes in the liquid phase as follows:

PARAMETER	EXPRESSION
α_1	10
α_2	3

You normally set initial conditions on the **Init** page. However, the default initial value for solute concentrations is zero, which is the value that applies here.

5 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions

1 From the **Physics** menu, select **Boundary Settings**.

2 Enter the following settings; when done, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARIES 2–4
Boundary condition	Concentration	Advective flux
c_0	0	

Point Settings

1 From the **Physics** menu, select **Point Settings**.

2 On the **Flux, c** page, select Point 3.

3 In the $\mathbf{N_0}$ edit field for the flux, type `c_s*W/b`.

4 In the $\mathbf{t_{Nf}}$ edit field for the ending time, type `360`.

5 Click **OK**.

MESH GENERATION

1 Select the menu item **Mesh>Free Mesh Parameters**.

2 Click the **Subdomain** tab, then select Subdomain 1. In the **Maximum element size** edit field enter `20`.

3 Click the **Point** tab. Select Point 3, then for **Maximum element size** enter `1`.

4 Click **OK**.

5 Go to the Main toolbar and click the **Initialize Mesh** button.

COMPUTING THE SOLUTION

The solution requires two steps: First solve for the steady-state solution to the flow problem; second solve the transient solute-transport model using the velocities from the flow solution.

To solve the flow problem, proceed as follows:

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Solve For** page, select **Darcy's Law (esdl)**; make sure it is the only application mode selected, then click **OK**.

3 Click the **Solve** button on the Main toolbar.

To solve for solute concentrations, continue with these steps:

1 Click the **Solver Parameters** button on the Main toolbar.

2 From the **Analysis** list, select **Transient**. To generate outputs in 10-day increments from time 0 to time 360, go to the **Times** edit field and enter `0:10:360`. Click **OK**.

3 Click the **Solver Manager** button on the Main toolbar.

4 On the **Solve For** page, select only **Solute Transport (esst)**. Click **OK**.

5 Click the **Restart** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 4-1 proceed as follows:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, go to the **Plot type** area and select the **Surface** and **Arrow** check boxes.

3 Click the **Surface** tab. On the **Surface Data** page, choose **Darcy's Law (esdl)>Hydraulic head** from the **Predefined quantities** list.

4 On the **Arrow** page, click the **Subdomain Data** tab. From the **Predefined quantities** list choose **Darcy's Law (esdl)>Velocity field**. Go to the **Arrow positioning** area, and in the **Number of points** edit fields for both **x points** and **y points** enter `15`. Click the **Color** button. Change the selection to black, then click **OK**.

5 Click **Apply** to generate the plot.

To generate the plot in the upper left panel of Figure 4-3, continue with these steps:

1 On the **General** page, find the **Plot type** area and clear the **Arrow** check box. In the **Solution at time** list select **30**.

2 Click the **Surface** tab. On the **Surface Data** page, enter `c*(c<50)+50*(c>=50)` in the **Expression** edit field. Click the **Range** button and clear the **Auto** check box. In the **Min** edit field enter `0.1`, and in the **Max** edit field keep the default value (**50**). Click **OK**.

3 Click **OK**.

To generate the other two plots, follow these steps:

1 Choose **Postprocessing>Plot Parameters** and click the **General** tab.

2 From the **Solution at time** list select **90**. Click **Apply**.

3 Repeat Step 2 but this time with a value of **360**.

To generate Figure 4-4 continue with these steps:

1 From the **Postprocessing** menu select **Cross-Section Plot Parameters**.

2 In the **Solution to use** list select **10, 30**, **90**, **180**, and **360**. (You can choose multiple solution times by pressing the Ctrl key.)

3 Click the **Line/Extrusion** tab. Go to the **y-axis data** area and from the **Predefined quantities** list choose **Solute Transport (esst)>Advective flux c**. Edit the resulting entry in the **Expression** edit field to read `adflux_c_esst/SPD`. Edit the entry in the **Unit** edit field to read `kg/(m^2*day)`. With these modifications, the *y*-axis gets the correct unit in the plot (recall the discussion under "Application Scalar Variables" on page 222).

4 In the **Cross-section line data** area, enter the following settings:

x_0	x_1	y_0	y_1
0	450	150	150

5 In the **x-axis data** area, click first the lower option button and then the **Expression** button. In the **X-Axis Data** dialog box, type `x` in the **Expression** edit field. Click **OK**.

6 Click **Apply**.

To generate Figure 4-5, continue with these steps:

1. From the **Postprocessing** menu select **Cross-Section Plot Parameters**.
2. Click the **Line/Extrusion** tab. Go to the **y-axis data** area and in the **Predefined quantities** list choose **Solute Transport (esst)>Dispersive flux, c**. Edit the resulting entry in the **Expression** edit field to read dflux_c_esst/SPD. Edit the entry in the **Unit** edit field to read kg/(m^2*day).
3. Click **OK**.

To generate Figure 4-6, proceed as follows:

1. From the **Options** menu select **Axes/Grid Settings**. Click the **Grid** tab and clear the **Auto** check box. Clear the **Auto** check box in the **z grid** area. In the **z spacing** edit field enter 10. Although *z* is not a model coordinate, you need *z* gridding to make a height plot. Click **OK**.
2. From the **Postprocessing** menu select **Plot Parameters**.
3. On the **General** page, click the **Title** button. In the edit field enter the title Solute concentrations in the range 0.1 ppm to 0.5 ppm [kg/m³]. Click **OK**.
4. Click the **Surface** tab. On the **Surface Data** page, the entry in the **Expression** edit field should read c_ppm*(c_ppm<50)+50*(c_ppm>=50). Click the **Range** button, then verify that the **Auto** box is cleared and that the settings are 0.1 for **Min** and 50 for **Max**. Click **OK**.
5. Still on the **Surface** page, click the **Height Data** tab and then select the **Height data** check box. In the **Expression** edit field use the same one as you entered on the **Surface Data** page. You can copy and paste the expression c_ppm*(c_ppm<50)+50*(c_ppm>=50) into the edit field.
6. Click **Apply**.
7. To view solutions for all time steps as a movie, click the **Animate** tab and then click the **Start Animation** button.

Buoyancy Flow with Darcy's Law—the Elder Problem

Density variations can initiate flow even in a still fluid. In earth systems, density variations can arise from naturally occurring salts, subsurface temperature changes, or migrating pollution. This buoyant or density-driven flow factors into fluid movement in salt-lake systems, saline-disposal basins, dense contaminant and leachate plumes, and geothermal reservoirs, to name just a few.

This example duplicates a benchmark problem for time-dependent buoyant flow in porous media. Known as the Elder problem (Ref. 1), it follows a laboratory experiment to study thermal convection. When Voss and Souza (Ref. 2) recast the Elder problem for salt concentrations, it became a benchmark that many researchers have used to test a number of variable-density flow codes including SUTRA (Ref. 3) and SEAWAT (Ref. 4).

This model examines the Elder problem for concentrations through a 2-way coupling of two application modes from the Earth Science Module: Darcy's Law and Solute Transport.

Model Definition

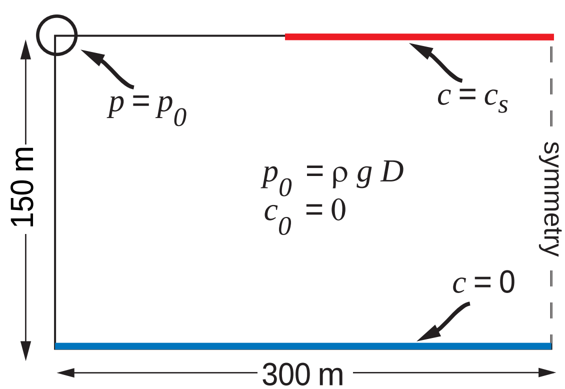


Figure 4-7: Geometry for modeling the Elder problem. In this cross section of water-saturated porous media, a high salt concentrations exist on the top right portion.

In this model (Figure 4-7) a vertical cross section of water-saturated porous media extends 300 m in the x direction and 150 m in the y direction. The material properties are homogeneous and isotropic. A vertical line at $x = 300$ m represents a symmetry boundary with a mirror image of the cross section extending beyond it. There is no flow across the geometry edges. High salt concentrations exist at the upper boundary (along $y = 150$ m) from $x = 150$ to 300 m. Salt concentration is zero along the lower boundary. The water is initially stationary (with a hydrostatic pressure distribution) and pristine (with zero concentration). When the density increases near the high-concentration boundary, flow develops. The period of interest is 20 years.

FLUID FLOW

You can describe the fluid flow in this problem using Darcy's law with an extra term:

$$\rho S\frac{\partial p}{\partial t} + \theta\frac{\partial \rho}{\partial c}\frac{\partial c}{\partial t} + \nabla \cdot \left[-\rho\frac{\kappa}{\eta}\nabla(p + \rho g D)\right] = 0$$

where the pressure, p (in units of $\mathrm{kg/(s^2{\cdot}m)}$), and the concentration, c ($\mathrm{kg/m^3}$), are dependent variables. In this equation ρ is the density ($\mathrm{kg/m^3}$); S is the storage coefficient ($\mathrm{s^2{\cdot}m^2/kg}$); t is the time; and θ is the porosity. The divergence operator has a velocity multiplied by a fluid density where κ equals the permeability ($\mathrm{m^2}$), η is the viscosity ($\mathrm{kg/(s{\cdot}m)}$), g is gravity ($\mathrm{m/s^2}$); and D is the vertical coordinate, y.

Now define density as a function of concentration according to

$$\rho = \rho_0 + \gamma(c - c_0) = \rho_0 + \frac{\rho_s - \rho_0}{c_s - c_0}(c - c_0) .$$

Multiplying the time-rate change in concentration by γ gives the change in mass stored per time as a function of concentration.

The density, ρ, appears as a multiplier to the time-rate change in pressure and also as a scalar multiplier of the velocity

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

where $\mathbf{u}$ is the vector of directional seepage rates, also known as Darcy velocities. Storage is negligible in the Elder problem, and storage changes come from variations in density as a function of concentration.

The symmetry or zero flow on all boundaries fix only the change in pressure. For a unique solution, you must also specify a reference pressure. In this case, choose a point. Then, with the Darcy's Law application mode, you express all these conditions as

$$\begin{array}{lll} \mathbf{n}\cdot\left[\frac{\kappa}{\eta}\nabla(p+\rho g D)\right]=0 & \partial\Omega & \text{Sides} \\ p=0 & \partial^2\Omega & \text{Point} \\ p(x,y,0)=\rho_0 g D & t=0 & \end{array}$$

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

SOLUTE TRANSPORT

The governing equation for this problem is the conservative form of the Solute Transport application mode

$$\theta_s\frac{\partial c}{\partial t}+\nabla\cdot[-\theta_s D_L\nabla c+\mathbf{u}c] = 0$$

where D_L is the hydrodynamic dispersion tensor (m^2/d); θ_s is the fluid volume fraction; c is the dissolved concentration (kg/m^3); $\mathbf{u}$ is the Darcy velocity (m/d); and S_c is the quantity of solute added per unit volume of porous medium per unit time (kg/m^3d).

In the Elder problem, the contaminant spreads only by advection and molecular diffusion. With a typical transport problem, the hydrodynamic dispersion tensor, D_L, also contains mechanical mixing owing to variations in velocity. The diagonal components, D_{Lii}, of the tensor are

$$\theta D_{Lii} = \alpha_1\frac{u_i^2}{|\mathbf{u}|}+\alpha_2\frac{u_j^2}{|\mathbf{u}|}+\tau D_m$$

where α is the dispersivity (m); the subscripts "1" and "2" denote longitudinal and transverse flow, respectively; τ is tortuosity; and D_m is the coefficient of molecular diffusion (m^2/s). Because the Elder problem requires diffusion alone, the first two terms in this expression equal zero.

The only contaminant source in the model domain is the salt concentration along the right half of the upper boundary. The vertical edge at x = 300 m is a symmetry boundary. The remaining boundaries have zero flux. The initial concentration is zero. The following equations represent these conditions:

$$\mathbf{n} \cdot [-\theta_s D_L \nabla c + \mathbf{u}c] = 0 \qquad \partial\Omega \quad \text{Sides}$$

$$c = c_s \qquad \partial\Omega \quad \text{Salt}$$

$$c(x, y, 0) = 0 \qquad t = 0$$

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

Data

The model works with the following data:

PARAMETER	NAME	VALUE
ρ_0	Fresh-water density	1000 kg/m^3
ρ_s	Salt-water density	1200 kg/m^3
κ	Permeability	$4.85 \cdot 10^{-13}$ m^2
η	Dynamic viscosity	0.001 kg/(m·s)
g	Gravity	9.81 m/s^2
θ_s	Porosity	0.1
τD_m	Molecular diffusion rate	$3.56 \cdot 10^{-6}$ m^2/s
c_s	Salt-water concentration	285.7 kg/m^3
c_0	Fresh-water concentration	0 kg/m^3

Results and Discussion

The following results come from the COMSOL Multiphysics solution to a benchmark buoyancy problem often used both for temperatures (Ref. 1) and concentrations (Ref. 2).

Figure 4-8 gives snapshots of concentrations at six times during the 20-year simulation period. Initially the water is pristine. By the end of the first year, concentrations spread by diffusion, creating a density gradient. The buoyancy flow begins at the edge of the salt contact, where there is a sharp contrast in fluid density. By the end of year three, the fingering of high concentrations into the reservoir is mature. By year 10, the salt concentrations have spread over roughly 60% of the model domain.

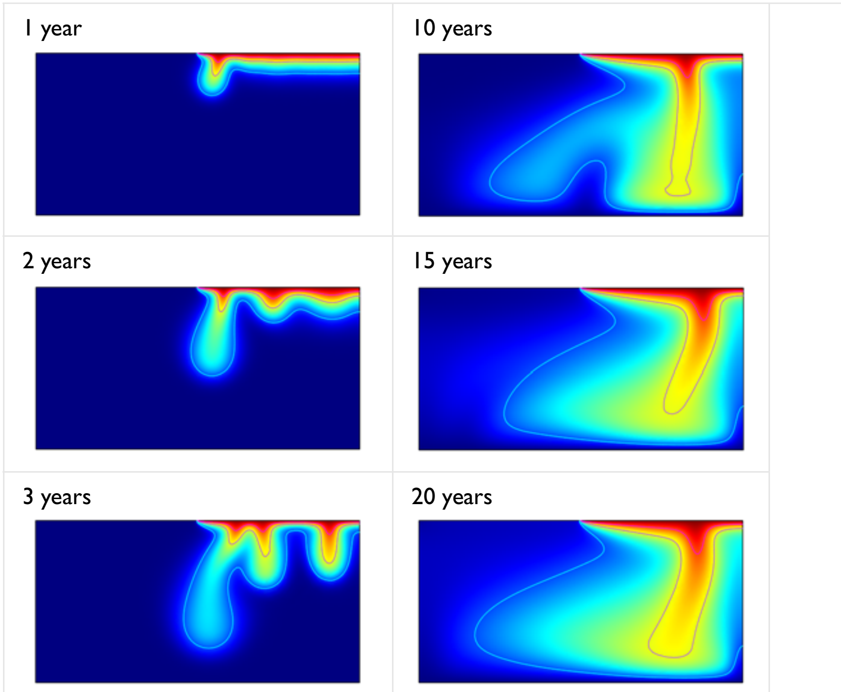


Figure 4-8: Snapshots of concentrations from the COMSOL Multiphysics *solution to the buoyancy-flow benchmark developed by Voss and Souza (Ref. 2) for the Elder problem.*

Figure 4-9 shows results from Elder (Ref. 1) along with numerical estimates from the SUTRA (Ref. 3) and SEAWAT (Ref. 4) manuals. The COMSOL Multiphysics solution in Figure 4-8 is in excellent agreement with that from Elder.

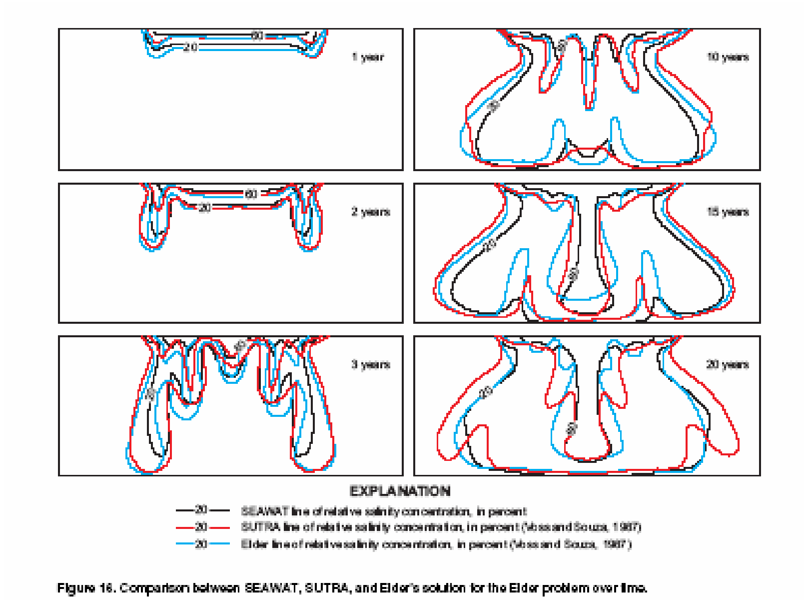


Figure 4-9: Results from the Elder problem shown with concentration estimates from SEAWAT and SUTRA (adapted from Ref. 4).

Of interest in the Elder problem is the development of convection cells. The COMSOL Multiphysics plots in Figure 4-10 reveal the convection cells with the help of velocity streamlines, which the figure shows simultaneously with concentrations for Years 5, 10, 15, and 20. At early times, small convection cells develop between the individual fingers of the plume. At late times, a single convection cell covers the model domain.

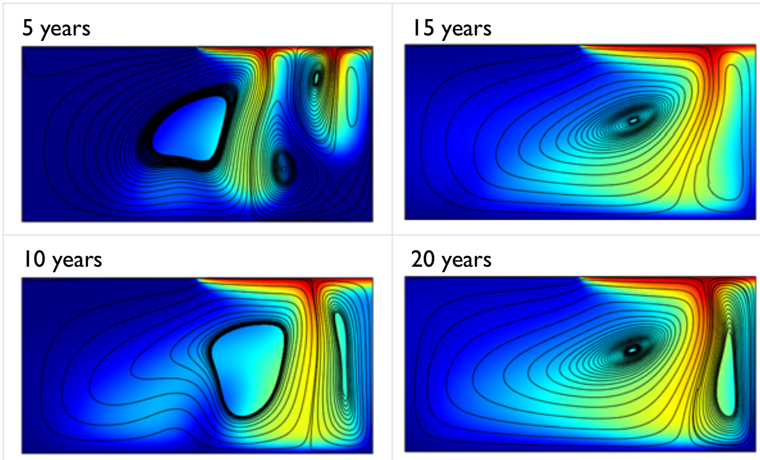


Figure 4-10: Salt concentrations (surface plot) and velocities (streamlines) from the COMSOL Multiphysics *solution to a buoyancy benchmark problem (Ref. 2).*

This example shows COMSOL Multiphysics applied to a well-known benchmark problem applicable to flow driven by density variations related to either temperature or concentration. The COMSOL Multiphysics results, here for concentration, closely match the benchmark solution (Ref. 2). This buoyant flow is straightforward to set up directly on top of a standard fluid flow and solute-transport model.

References

1. J.W. Elder, "Transient convection in a porous medium," *J. Fluid Mechanics*, vol. 27, no. 3, 1967.

2. C.I. Voss and W.R. Souza, "Variable density flow and solute transport simulation of regional aquifers containing a narrow freshwater-saltwater transition zone," *Water Resources Research*, vol. 23, no. 10, 1987.

3. C.I. Voss, A finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport, U.S. Geological Survey Water-Resources Investigation Report 84-4369, 198.

4. W. Guo and C.D. Langevin, *User's Guide to SEAWAT: A Computer Program for Simulation of Three-Dimensional Variable-Density Ground-Water Flow*, U.S. Geological Survey Techniques of Water-Resources Investigations 6-A7, 2002.

Model Library path: `Earth_Science_Module/Solute_Transport/buoyancy_darcy_elder`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Open the **Model Navigator**, click the **New** tab, and in the **Space dimension** list select **2D**.

2 From the list of application modes choose **Earth Science Module>Fluid Flow>Darcy's Law>Pressure analysis>Transient analysis**.

3 Click the **Multiphysics** button. Click **Add**.

4 From the list of application modes choose **Earth Science Module>Solute Transport>Saturated Porous Media>Transient analysis**. Click **Add**.

5 Click the **Application Mode Properties** button.

6 In the **Equation form** list select **Conservative** (this step moves the velocity term inside the divergence operator). In the **Material** list select **Liquid**. Click **OK**.

7 Click **OK**.

GEOMETRY MODELING

1 Select the menu item **Draw>Specify Objects>Rectangle**

2 In the dialog box that opens, go to the **Width** edit field and enter `300`, and for the **Height** enter `150`. Click **OK**.

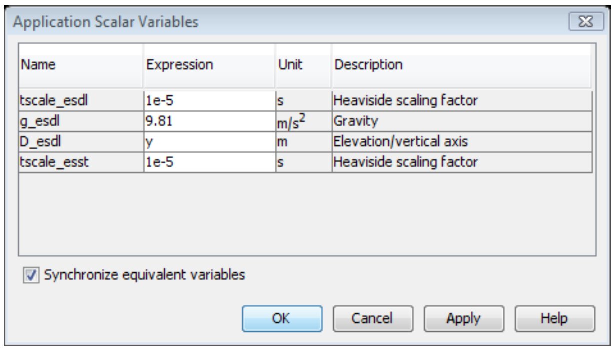
3 Click the **Zoom Extents** button on the Main toolbar to center the rectangle in the field of view.

4 From the **Options** menu select **Axes/Grid Settings**. Click the **Grid** tab and clear the **Auto** check box. In the **Extra x** edit field enter `150`, and in the **Extra y** edit field enter `150`. Click **OK**.

5 Select the menu item **Draw>Specify Objects>Line**. To draw a line from (x, y) = (150, 150) to (300, 150) enter space-separated values: for **x coordinates** enter `150 300`, and for **y coordinates** enter `150 150`.

APPLICATION SCALAR VARIABLES

The **Darcy's Law (esdl)** application mode assumes that gravity **g_esdl** equals 9.82 m/s^2 and that the vertical dimension **D_esdl** is the screen's y-axis. To set up these conditions, select the menu item **Physics>Scalar Variables**. In the **g_esdl** edit field enter `9.81`, and for **D_esdl** enter `y`. Click **OK**.

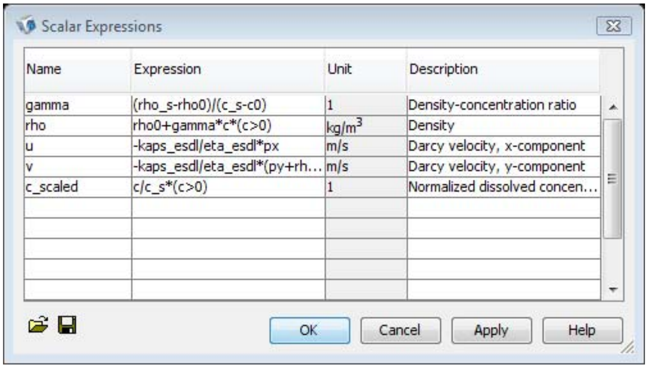


OPTIONS AND SETTINGS

1 From the **Options** menu choose **Constants**. Then enter the following names, expressions, and (optionally) descriptions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
`rho0`	`1000[kg/m^3]`	`Fresh-water density`
`rho_s`	`1200[kg/m^3]`	`Salt-water density`
`kappa`	`4.85e-13[m^2]`	`Permeability`
`eta`	`0.001[kg/(m*s)]`	`Dynamic viscosity`
`theta_s`	`0.1`	`Porosity`
`tauD_m`	`3.56e-6[m^2/s]`	`Molecular diffusion rate`
`c_s`	`285.7[kg/m^3]`	`Salt-water concentration at upper right boundary`
`c0`	`0[kg/m^3]`	`Fresh-water concentration at upper right boundary`

2 From the **Options** menu select **Expressions>Scalar Expressions**. Enter the following names, expressions, and descriptions; when done, click **OK**.



NAME	EXPRESSION	DESCRIPTION
gamma	(rho_s-rho0)/(c_s-c0)	Density-concentration ratio
rho	rho0+gamma*c*(c>0)	Density
u	-kaps_esdl/eta_esdl*px	Darcy velocity, x-component
v	-kaps_esdl/eta_esdl*(py+rho*g_esdl)	Darcy velocity, y-component
c_scaled	c/c_s*(c>0)	Normalized dissolved concentration

PHYSICS SETTINGS—DARCY'S LAW

To set up the flow model, perform these steps: activate the Darcy's Law application mode; enter material properties for the subdomain; insert the varying density as a scaling term; give the boundary conditions; and then add to the equation the time change in density with concentration.

Multiphysics

From the **Multiphysics** menu select **Darcy's Law (esdl)**.

Subdomain Settings

1 From the **Physics** menu select **Subdomain Settings**. Select Subdomain 1.

2 On the **Coefficients** page, enter the following values:

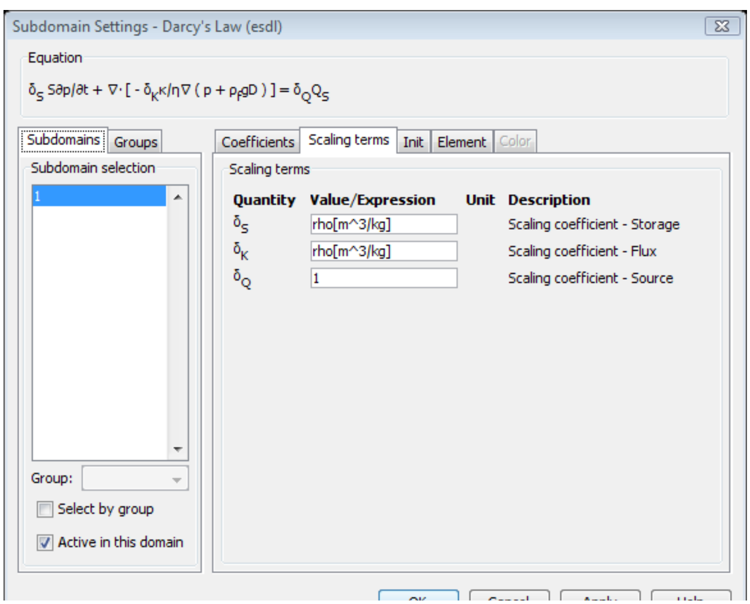
PROPERTY	VALUE
S	`eps`
κ_s	`kappa`
ρ_f	`rho`
η	`eta`
Q_s	`0`

Here, you use the machine precision constant `eps` to get a small transient term that helps the solver to converge on a solution. The term is small enough that it has no effect on the solution obtained.

3 On the **Scaling terms** tab, enter the following settings:

PROPERTY	VALUE
δ_S	`rho[m^3/kg]`
δ_K	`rho[m^3/kg]`

Note that these settings only scale the complete equation by an overall factor (δ_Q is irrelevant because this model does not include a distributed source). This is done to improve convergence.



4 On the **Init** page, define the initial hydrostatic pressure distribution by entering `rho0*g_esdl*(150[m]-y)` in the **p(t_0)** edit field.

5 Click **OK**.

Boundary Conditions

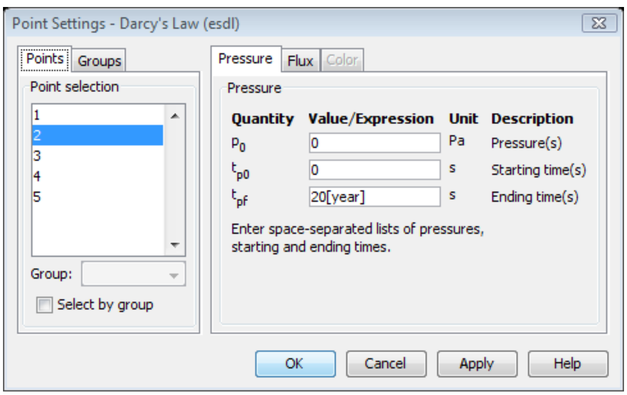
From the **Physics** menu select **Boundary Settings** and verify that all the boundaries (numbers 1 through 5) are no-flow; for each boundary, the entry in the **Boundary condition** list should read **Zero flux/Symmetry**. When done, click **OK**.

Point Settings

With all boundaries being flux statements, you must set the pressure at a point to get a unique solution.

1 From the **Physics** menu select **Point Settings**.

2 In the resulting dialog box click the **Pressure** tab. In the **Point selection** list select **2**. For the two variables $\mathbf{p_0}$ and $\mathbf{t_{p0}}$ to go the corresponding **Value/Expression** edit fields and enter `0`. Then, in the **Value/Expression** edit field for $\mathbf{t_{pf}}$ enter `20[year]`. Click **OK**.



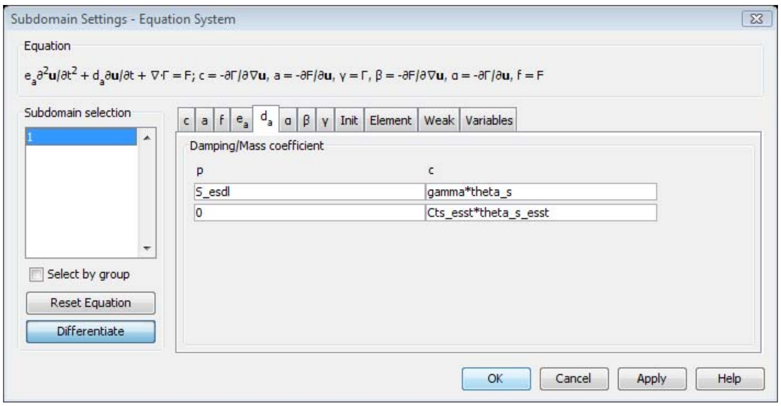
Equation System Settings

1 Select the menu item **Physics>Equation System>Subdomain Settings.** Here you enhance the flow equation with the time change in density with concentration. Entries in the **Subdomain Settings - Equation System** dialog box actually change the way that COMSOL Multiphysics solves a problem, so following any changes, COMSOL Multiphysics displays a lock on the subdomain number.

2 Click the $\mathbf{d_a}$ tab to go where COMSOL Multiphysics picks up coefficients that multiply the time change in the dependent variables in this problem. Edit the mass-coefficient entries so they read as follows:

P	C
`S_esdl`	`gamma*theta_s`
`0`	`Cts_esst*theta_s_esst`

3 Click the **Differentiate** button to distribute the change throughout the equation system.



4 Click **OK**.

PHYSICS SETTINGS—SOLUTE TRANSPORT

To set up the solute-transport model, you activate the application mode, enter material and solute properties for the subdomain, and specify boundary conditions. You must also change how COMSOL Multiphysics defines the dispersion tensor to exclude mechanical mixing.

Multiphysics

From the **Multiphysics** menu select **Solute Transport (esst)**.

Subdomain Settings

1 From the **Physics** menu select **Subdomain Settings**.

2 Next specify the flow field and the velocities you defined earlier in the **Options>Expressions>Scalar Expressions** dialog box. You do not use the predefined velocities **u_esdl** and **v_esdl** from the **Darcy's Law (esdl)** application mode. The reason

is that with the extra density term added inside the divergence operator, the predefined variables now represent mass flux instead of velocity.

In the **Subdomain Settings** dialog box go to **Subdomain selection** list and make sure **1** is selected. Click the **Flow and Media** tab. Enter the expressions in the following table; when finished, click **Apply**.

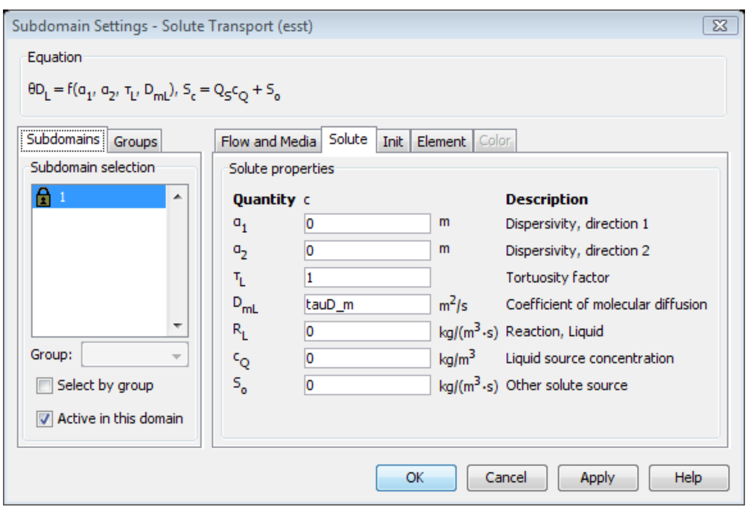
PROPERTY	VALUE
θ_s	`theta_s`
u	u
v	v

3 Click the **Solute** tab to set the dispersivities that describe spreading for solutes in the liquid phase. Enter the expressions in the following table; when done, click **Apply**.

PROPERTY	VALUE
α_1	0
α_2	0
T_L	1
D_{mL}	`tauD_m`

4 You can always set initial conditions by going to the **Init** page. However, the default initial value for solute concentrations is zero, which is the value needed here.

5 Click **OK**.



Boundary Conditions

From the **Physics** menu select **Boundary Settings**. Set the conditions and enter expressions for the various boundaries as in this table; when done, click **OK**.

SETTINGS	BOUNDARY 2	BOUNDARY 4	BOUNDARIES 1, 3, 5
Type	Concentration	Concentration	No flux/Symmetry
c_0	c0	c_s	

Equation System Settings

1 Select the menu item **Physics>Equation System>Subdomain Settings**, then click the **Variables** tab. Here you change the preset definitions for application-mode variables dictating how COMSOL Multiphysics calculates the entries of the dispersion tensor.

2 Scroll down the list of predefined variables until you find the following and edit them so they read as follows:

NAME	EXPRESSION
thDLxx_c_esst	theta_s_esst*tauL_c_esst*DmL_c_esst
thDLxy_c_esst	0
thDLyx_c_esst	0
thDLyy_c_esst	theta_s_esst*tauL_c_esst*DmL_c_esst

3 Click **Differentiate**, then click **OK**.

MESH GENERATION

1 From the **Mesh** menu select **Free Mesh Parameters**.

2 In the resulting dialog box, click the **Global** tab. In the list of **Predefined mesh sizes** select **Fine**, then click the **Custom mesh size** button and in the **Element growth rate** edit field enter 1.15.

3 Switch to the **Boundary** page, then select boundaries **1**, **3**, and **5**. In the **Maximum element size** edit field enter 10. For boundary **2** enter a **Maximum element size** of 7. For boundary **4** enter a **Maximum element size** of 5.

4 Click the **Point** tab, select point **3**, and enter a **Maximum element size** of 1. For point **5** enter a **Maximum element size** of 3.

5 Click **Remesh**. Click **OK**.

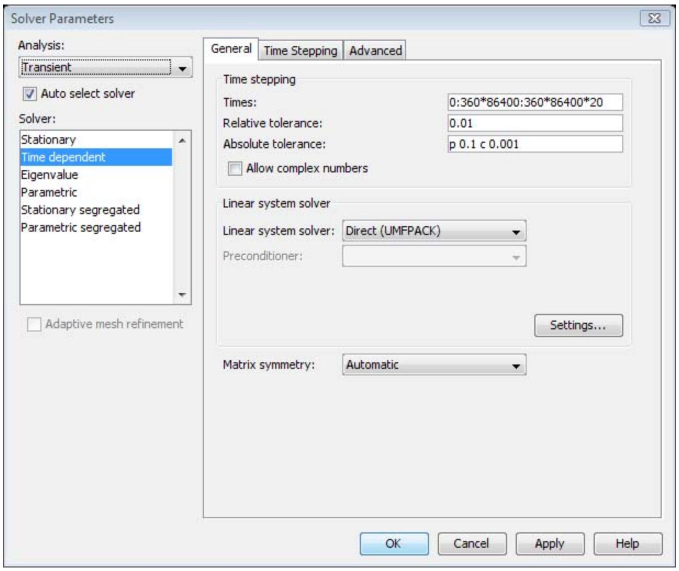
COMPUTING THE SOLUTION

COMSOL Multiphysics solves the flow and transport problems simultaneously.

1 From the **Solve** menu choose **Solver Parameters**. Look in the **Solver** list and verify that the **Time dependent** solver is selected.

2 Find the **Times** edit field and enter `0:360*86400:360*86400*20` to generate outputs from 0 to 20 years in 1-year increments.

3 As the **Absolute tolerance** expression enter `p 0.1 c 0.001`. Doing so sets a different error tolerance for pressure than concentration because their magnitudes differ significantly. Click **OK**.



4 Click **Solve** on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the images in Figure 4-8 proceed as follows:

1 From the **Postprocessing** menu select **Plot Parameters**.

2 Click the **General** tab, and in the **Plot type** area select the **Surface** and **Arrow** check boxes. Go to the **Solution at time** list and choose a time of interest. Click **Apply**.

3 Go to the **Surface** tab and then to the **Surface Data** page. In the **Expression** edit field type `cscaled`.

4 Click the **Contour** tab. Select the **Contour plot** check box. On the **Contour Data** page**,** go to the **Expression** edit field and enter `c_scaled` as before.

5. Go to the **Contour levels** area. Select the **Vector with isolevels** option button, and in the corresponding edit field enter `0.2 0.6 0.8`. Click **Apply**.
6. To view the solutions for all time steps as a movie, go to the **Animate** tab and click **Start Animation**.

To generate the images in Figure 4-10, follow these steps:

1. From the **Postprocessing** menu choose **Plot Parameters**.
2. Click the **General** tab. In the **Plot type** area, clear the **Contour** check box and select the **Streamline** check box. Make a selection in the **Solution at time** list as desired.
3. Click the **Streamline** tab and then go to the **Streamline Data** page. In the **x component** edit field overwrite the default value with `u`, and in the **y component** edit field enter `v`.
4. From the **Streamline plot type** list, select **Magnitude controlled**. On the **Density** page, set the **Density** to `10`.
5. Click the **Line Color** tab. Click the **Uniform color** option button, then click the **Color** button. In the **Streamline Color** dialog box, select black, then click **OK**.
6. Click **Apply** to generate the first plot.
7. Return to the **General** page and select the desired solutions in the **Solution at time** list, clicking **Apply** inbetween to generate the plots.
8. To view solutions for all time steps as a movie, go to the **Animate** page and click **Start Animation**.

Variably Saturated Flow and Transport

This example details two assessments of time-dependent fluid flow and solute transport for a variably saturated system. In the first transport scenario, "Sorbing Solute," a chemical sorbs to soil particles and biodegrades. In the second scenario, section "Pesticide Transport and Reaction in Soil", the pesticide aldicarb transforms to daughter products that you then track. The inspiration for the two problems comes from the manuals of SWMS2D (Ref. 1) and HYDRUS2D (Ref. 2).

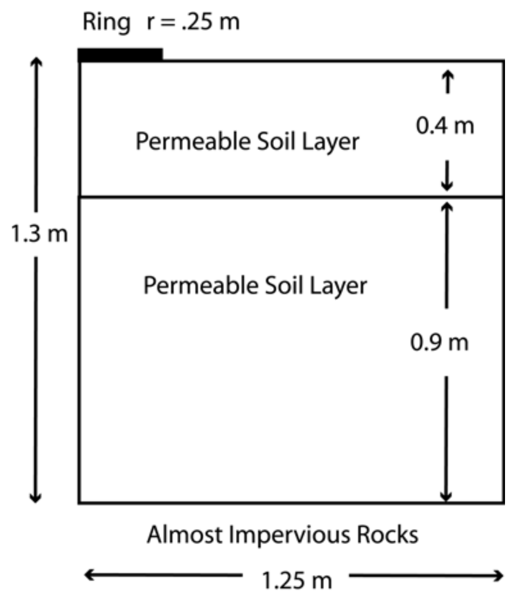


Figure 4-11: Geometry of the infiltration ring and soil column.

The two chemical-transport scenarios from this example build on top of the same variably saturated flow model. It uses the Richards' equation interfaces to define nonlinear relationships with retention and permeability properties according to van Genuchten (Ref. 3). In the Richards' Equation application mode you can also define these material properties by interpolation from experimental data (see "Interpolation for Unsaturated Flow" on page 115) and the Brooks and Corey analytic permeability and retention formulas (Ref. 4).

The two variably saturated flow and solute-transport models included here are inspired by but do not exactly duplicate the SWMS2D and HYDRUS2D examples. The main distinction lies in the governing equations. SWMS2D and HYDRUS2D use a form of Richards' equation that accounts for change in fluid volume fraction with time. The Richards' Equation application mode also accounts for changes in storage related to variations in pressure head according to Bear (Ref. 5) among others. Another point of departure is that with the storage terms, the solute-transport equations in the Earth Science Module also account explicitly for time change in liquid and air content. Moreover, the problems here address isothermal conditions. For nonisothermal flow see "Free Convection in Porous Media" on page 294.

Model Definition—Sorbing Solute

In the fluid-flow model, water moves from a ring on the ground into the subsurface. The 0.25-m radius ring ponds the water to a depth of 0.01 m but is open to the ground surface. Permeable soils exist to a depth of 1.3 m. The soil in the uppermost 0.4 m is slightly less permeable than the 1.9 m below it. The lower layer sits above relatively impermeable soil, so only a very small amount of leakage exits from the base. The flow is symmetric about the line $x = 0$. No flow crosses the surface outside the ring. According to the problem statement there is no flow across the line $x = 1.25$ m. The initial distribution of pressure heads is known.

The water in the ring contains a dissolved solute at a constant concentration, c_0. The solute enters the ground with the water and moves through the subsurface by advection and dispersion. Additionally, the solute sorbs or attaches to solid surfaces, which reduces the aqueous concentrations and also slows solute movement relative to the water. Microbial degradation also reduces both the liquid- and the solid-phase concentrations. The sorption and the biodegradation are linearly proportional to aqueous concentrations. The fluid in the ring is the only chemical source, and the solute is free to leave the soil column with the fluid flux. Initially the soil is free of the solute. You track its transport for ten days.

FLUID FLOW

Richards' equation governs the saturated-unsaturated flow of water in the soil. The soil air is open to the atmosphere, so you can assume that pressure changes in air do not affect the flow and use Richards' equation here for single-phase flow. Given by Ref. 5, Richards' equation reads

$$[C + \mathrm{Se}S]\frac{\partial H_p}{\partial t} + \nabla \cdot [-K_s k_r \nabla(H_p + D)] = Q_s$$

where C denotes specific moisture capacity (m^{-1}); Se is the effective saturation of the soil; S is a storage coefficient (m^{-1}); H_p represents the dependent variable pressure head (m); t is time (d); K equals the hydraulic conductivity function (m/d); D is the coordinate (for example, x, y, or z) that represents vertical elevation, and Q_s is a fluid source defined by volumetric flow rate per unit volume of soil (d^{-1}). In this problem, $S = \theta_\mathrm{s} - \theta_\mathrm{r}$ where θ_s and θ_r denote the volume fraction of fluid at saturation and after drainage, respectively.

With variably saturated flow, fluid moves through but may or may not completely fill the pores in the soil, and θ denotes the volume fraction of fluid within the soil. C, Se, and K vary with the pressure head, H_p, and with θ, making Richards' equation nonlinear. The specific moisture capacity, C, relates variations in soil moisture to pressure head as in $C = \partial\theta/\partial H_p$. In the governing equation, C defines storage changes produced by varying fluid content because $C\partial H_p/\partial t = \partial\theta/\partial t$. Because C, the first term in the bracketed time coefficient, goes to zero at saturation, time change in storage relates to compression of the aquifer and water under saturated conditions. The saturated storage comes about with the effective saturation as represented by the second term in the time-coefficient brackets. K is a function that defines how readily the porous media transmits fluid. The relative permeability of the soil, k_r, increases with fluid content giving $K = K_s\, k_r$, where K_s (m/d) is the constant hydraulic conductivity at saturation.

This example uses predefined interfaces for van Genuchten (Ref. 3) formulas to represent how the four retention and permeability properties θ, C, Se, and $k_r = K_s/K$ vary with the solution H_p. The van Genuchten expressions read as follows:

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

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

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

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

where α, n, m, and l are dimensionless constants that specify a particular media type, and $m = 1–1/n$. In the equations, the system reaches saturation when fluid pressure is atmospheric (that is, $H_p = 0$). When the soil fully saturates, the four parameters reach constant values.

The problem statement records all the boundary conditions you need for this model. The level of water in the ring is known at 0.01 m, giving a Dirichlet constraint on pressure head. Approximate the small leak from the base, N_0, as $0.01K_s$. With no flow crossing the surface outside of the pressure ring or the vertical walls, the following expressions summarize the boundary conditions:

$$\begin{aligned} &H_p = H_{p0} && \partial\Omega \ \text{Ring} \\ &\mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = 0 && \partial\Omega \ \text{Surface} \\ &\mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = 0 && \partial\Omega \ \text{Sides} \\ &\mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = 0 && \partial\Omega \ \text{Symmetry} \\ &\mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = N_0 && \partial\Omega \ \text{Base} \end{aligned}$$

In these expressions, $\mathbf{n}$ is the unit normal to the bounding surface.

A unique solution to a time-dependent problem requires an initial condition. In the problem statement, the initial condition came from results of another simulation. For this example model, you fit a simple equation to the June 1982 results shown in Example 4 from SWMS2D (Ref. 1) and run a short simulation without the ring to warm up the flow field. That simulation also assumes that there is no flow across the surface beneath the ring.

MULTIPHYSICS COUPLING

Groundwater flow and solute transport are linked by fluid velocities. With the form of the transport equation that follows, the fluid velocities need come from Darcy's law.

$$\mathbf{u} = K_s k_r \nabla(H_p + D) \tag{4-1}$$

In the expression, $\mathbf{u}$ is a vector of directional velocities often termed specific discharge (m/d). In COMSOL Multiphysics, u and v denote the velocities in the x and y directions, respectively, that make up $\mathbf{u}$.

SOLUTE TRANSPORT

The equation that governs advection, dispersion, sorption, and decay of solutes in groundwater is

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_b c_P) = \nabla \cdot [-\theta D_L \nabla c + \mathbf{u}c] = \Sigma R_L + \Sigma R_P + S_c$$

It describes time rate change in two terms: c denotes dissolved concentration (kg/m), and c_P is the mass of adsorbed contaminant per dry unit weight of solid (mg/kg). Further, θ denotes the volume fluid fraction (dimensionless), and ρ_b is the bulk density (kg/m^3). Because ρ_b amounts to the dried solid mass per bulk volume of the solids and pores together, the term $\rho_b c_P$ gives solute mass attached to the soil as a concentration. In the equation, D_L is the hydrodynamic dispersion tensor (m^2/d); R_L represents reactions in water (kg/(m^3·d)); and R_L equals reactions involving solutes attached to soil particles (kg/(m^3·d)). Finally, S_c is solute added per unit volume of soil per unit time (kg/(m^3·d)).

It is far more convenient to solve the above equation only for dissolved concentration. This requires expanding the left side to

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_b c_P) = \theta\frac{\partial c}{\partial t} + c\frac{\partial \theta}{\partial t} + \rho_b \frac{\partial c_P}{\partial c}\frac{\partial c}{\partial t}\,.$$

and inserting a few definitions.

In this problem, solute mass per solid mass, c_P, relates to dissolved concentration, c, through a linear isotherm or partition coefficient k_P (m^3/kg) where $c_P = k_P c$. Because the relationship is linear, the derivative is $k_p = \partial c_P / \partial c$. Making those substitutions gives the form of the solute transport problem you solve:

$$[\theta + \rho_b k_p]\frac{\partial c}{\partial t} + c\frac{\partial \theta}{\partial t} + \nabla \cdot [-\theta D_L \nabla c + \mathbf{u} c] = \theta \phi_L c + \rho_\mathrm{b} k_p \phi_P c + S_c \,.$$

In the equation, ϕ_L and ϕ_P denote the decay rates (d^{-1}) for the dissolved and sorbed solute concentrations, respectively.

Note that you employ results from the flow equation in the solute-transport model as

$$c\frac{\partial \theta}{\partial t} = cC\frac{\partial H_p}{\partial t} \,.$$

You enter this directly into the COMSOL Multiphysics user interface using the time-rate change in pressure head. Note that COMSOL Multiphysics solves for pressure, p, and converts to H_p based on the fluid weight.

The hydrodynamic dispersion tensor, D_L, describes mechanical spreading from groundwater movement in addition to chemical diffusion:

$$\theta D_{Lii} = \alpha_1 \frac{u_i^2}{|\mathbf{u}|} + \alpha_2 \frac{u_j^2}{|\mathbf{u}|} + \theta D_\mathrm{m} \tau_L$$

$$\theta D_{Lij} = \theta D_{Lji} = (\alpha_1 - \alpha_2)\frac{u_i u_j}{|\mathbf{u}|}$$

where D_{Lii} are the diagonal entries in the dispersion tensor; D_{Lji} and D_{Lji} are the cross terms; α is the dispersivity (m); the subscripts “1” and “2” denote longitudinal and transverse flow, respectively; D_m denotes the coefficient of molecular diffusion (m^2/d); and τ_L is a tortuosity factor that reduces impacts of molecular diffusion for porous media relative to free water. Here $\tau_L = \theta^{7/3} \theta_\mathrm{s}^{-2}$.

The boundary and initial conditions in the sorbing-solute problem are straightforward. The solute enters only with the water from the ring at a concentration c_0. The solute is free to leave, but there is only minimal leakage from the lower boundary and no flow from the sides. Transport is symmetric about the line $x = 0$. The boundary conditions in this problem are:

$$
\begin{array}{ll}
c = c_0 & \partial\Omega \ \text{Ring} \\
\mathbf{n} \cdot [-\theta D_L \nabla c] = 0 & \partial\Omega \ \text{Surface} \\
\mathbf{n} \cdot [-\theta D_L \nabla c] = 0 & \partial\Omega \ \text{Sides} \\
\mathbf{n} \cdot [-\theta D_L \nabla c + \mathbf{u} c] = 0 & \partial\Omega \ \text{Symmetry} \\
\mathbf{n} \cdot [-\theta D_L \nabla c] = 0 & \partial\Omega \ \text{Base}
\end{array}
$$

where **n** is the normal to the boundary. Because the soil is pristine at the start of the experiment, the initial condition is one of zero concentration.

IMPLEMENTATION—LOGICAL OPERATORS

This analysis uses logical operators to "warm up" the flow model for 0.1 days. The warm-up time smooths out the approximate equation for initial head to produce the smoothly varying, physically based velocity field needed to yield reasonable solute concentrations. You can use the **Solver Parameters** and **Solver Manager** dialog boxes to run a warm-up flow simulation first and use those results as initial conditions in the coupled-flow and transport problem as a follow-up step. The virtue of using logical operators here is that they circumvent the staged or multistep process.

Logical statements involve relational operators, which can be powerful tools for modeling in COMSOL Multiphysics. Multiplication of a constant or expression by a logical statement qualifies when, where, and how a model uses that expression or constant. For example, specifying c as `c0*(t>1)` means that the concentration equals `c0` for all times greater than 1, whereas multiplication by `(t>1)*(t<5)` means all times between $t = 1$ and $t = 5$.

This model uses the logical expressions as boundary conditions. For the flow problem, you need zero flow across the boundary during the warm-up time and a constant pressure head of 0.01 m thereafter. If you start the simulation at $t = -0.1$ days, you then turn on the constant pressure head and concentration at the ring at $t = 0$ with these equations:

$$
H_p \begin{cases} -\mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = 0 & t < 0 \\ H_p = 0.01 & 0 \le t \end{cases} \quad \partial\Omega \ \text{Ring}
$$

$$
c \begin{cases} \mathbf{n} \cdot (\theta_s D_L \nabla c - \mathbf{u} c) = 0 & t < 0 \\ c = 1 & 0 \le t \end{cases} \quad \partial\Omega \ \text{Ring}
$$

Using logical operators, you can implement the expressions for pressure head. Use the general Neumann boundary condition

$$-\mathbf{n} \cdot [-K_s k_r \nabla(H_p + D)] = q_0 + R_b[(H_{pb} - H_p) + (D_b - D)] .$$

On the right side of the equation, H_p is the solution, D is the current elevation, and all other terms are constants that you can define arbitrarily. Here set $q_0 = 0$, $R_b = 1$, $H_{Pb} = 0.01$, and $D_b = D$ for $t > 0$ by multiplication with logical operators. `Hpb=0.01*(t>=0)` means H_{Pb} has a value of 0.01 for all times greater than or equal to zero.

For concentration, use modified logic with the flux boundary expression

$$\mathbf{n} \cdot (\theta_s D_L \nabla c - \mathbf{u}c) = N_0 .$$

During the flow model's warm-up there is no solute moving from the pressure ring $N_0 = 0$. This is a Neumann condition on flux. Throughout the coupled-flow and transport problem, however, the solute concentration $c_{\text{ring}} = 1$, which is a Dirichlet condition on concentration. The logical operators use what is known as a "stiff-spring" condition to implement the switch between the two boundary types.

IMPLEMENTATION—STIFF-SPRING CONDITION

A stiff-spring condition uses weighting to make a Neumann statement about flux but achieves a Dirichlet condition on pressure head. The stiff-spring expression

$$\mathbf{n} \cdot [\theta_s D_L \nabla c - \mathbf{u}c] = N_0 = 10^6(c_{\text{ring}} - 1)$$

specifies the flux using a heavily weighted equivalence for concentration. Rephrased, the stiff-spring statement

$$c_{\text{ring}} = 1 + \mathbf{n} \cdot \frac{[\theta_s D_L \nabla c - \mathbf{u}c]}{10^6}$$

sets c_{ring} to 1 plus some small number. Because this offers virtually no information about the flux, it varies freely. In this model, set $N_0 = 10^6(c - 1)(t \geq 0)$.

DATA

The following table provides data for the fluid-flow model:

VARIABLE	UNIT	DESCRIPTION	UPPER LAYER	LOWER LAYER
K_s	m/d	Saturated hydraulic conductivity	0.298	0.454
θ_s	-	Porosity/void fraction	0.399	0.339
θ_r	-	Residual saturation	0.0001	0.0001
α	m^{-1}	alpha parameter	1.74	1.39
n	-	n parameter	1.38	1.60
m	-	m parameter	1-1/n	1-1/n
l	-	Pore connectivity parameter	n/a	
H_{ps}	m	Pressure head in ring	0.01	
H_{p0}	m	Initial pressure head	-(y+1.2)* (y<-0.4)+ (-(y+1.2)-0.2* (y+0.4))* (-0.4<=y)	-(y+1.2)* (y<-0.4)+ (-(y+1.2)-0.2* (y+0.4))* (-0.4<=y)

The inputs needed for the solute-transport model are:

VARIABLE	UNITS	DESCRIPTION	VALUE
r_b	kg/m^3	Bulk density	1400
k_p	m^3/kg	Partition coefficient	0.0001
D_m	m^2/d	Coefficient of molecular diffusion	0.00374
τ_L	-	Tortuosity factor	$\theta^{7/3}\theta_s^{-2}$
α_1	m	Longitudinal dispersivity	0.005
α_2	m	Transverse dispersivity	0.001
ϕ_L	d^{-1}	Decay rate in liquid	0.05
ϕ_P	d^{-1}	Decay rate on solid	0.01
c_s	kg/m^3	Solute concentration in ring	1.0
c_0	kg/m^3	Initial solute concentration in soil	0

Results

Figure 4-12 and Figure 4-13 give the solution to the fluid-flow problem at 0.3 and 1 day, respectively. The images show effective saturation (surface plot), pressure head (contours), and velocities (arrows). The figures illustrate the soil wetting with time. As the arrows indicate, the velocities just below the ring are high relative to the remainder of the soil column.

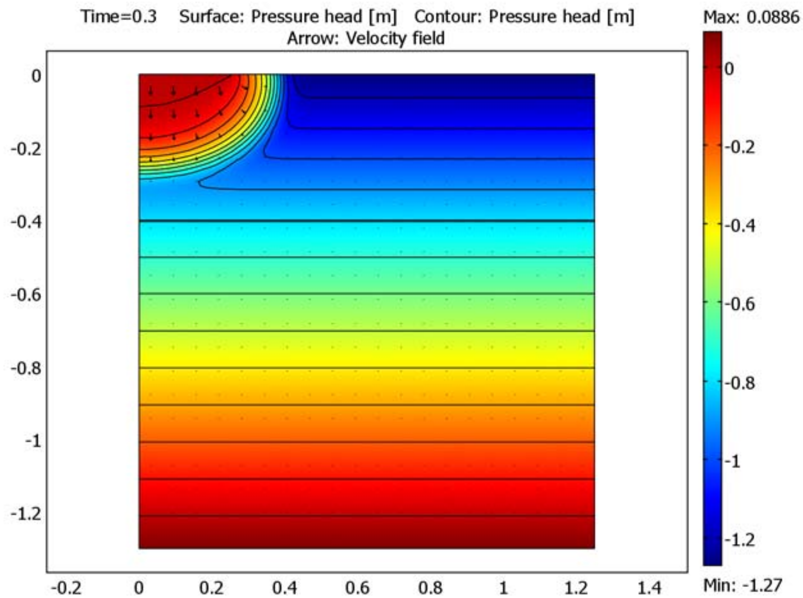


Figure 4-12: Estimates of effective saturation (surface plot), pressure head (contours), and velocity (arrows) in variably saturated soil after 0.3 days.

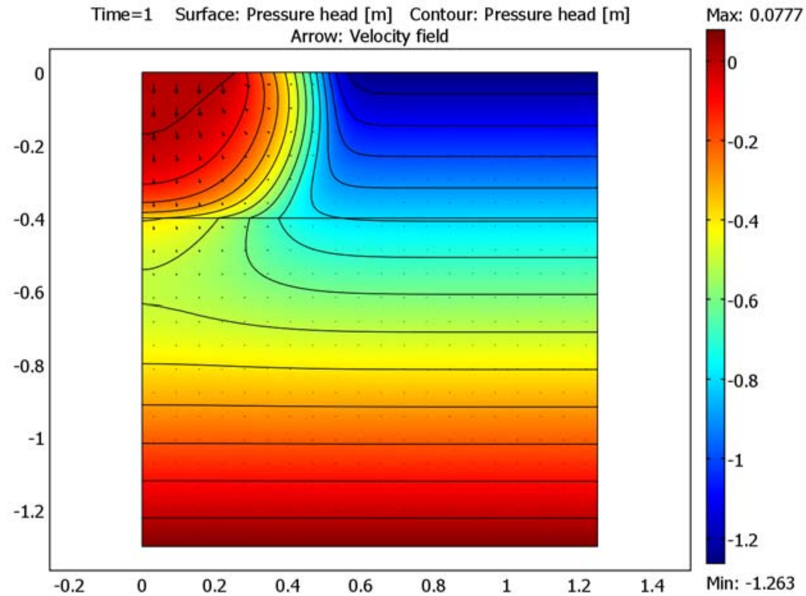


Figure 4-13: Estimates of effective saturation (surface plot), pressure head (contours), and velocity (arrows) in variably saturated soil after 1 day.

Figure 4-14 and Figure 4-15 give the concentrations for 0.25 days and 1 day, respectively, along with the retardation factor. They illustrate how the solute concentrations (surface plot) enter and move through the soil. Because the retardation factor depends on soil moisture, its value varies with the solution.

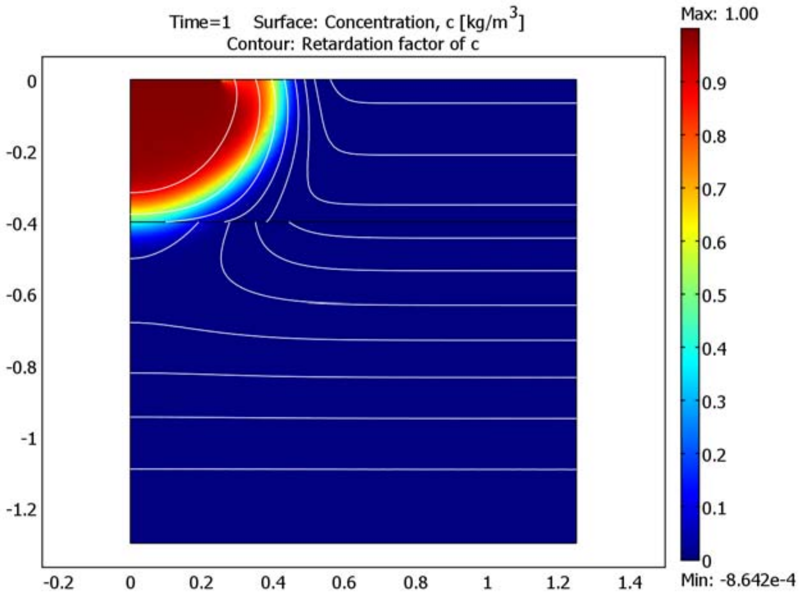


Figure 4-14: Solution for dissolved concentrations (surface plot) and retardation factor (contours) at 0.3 days.

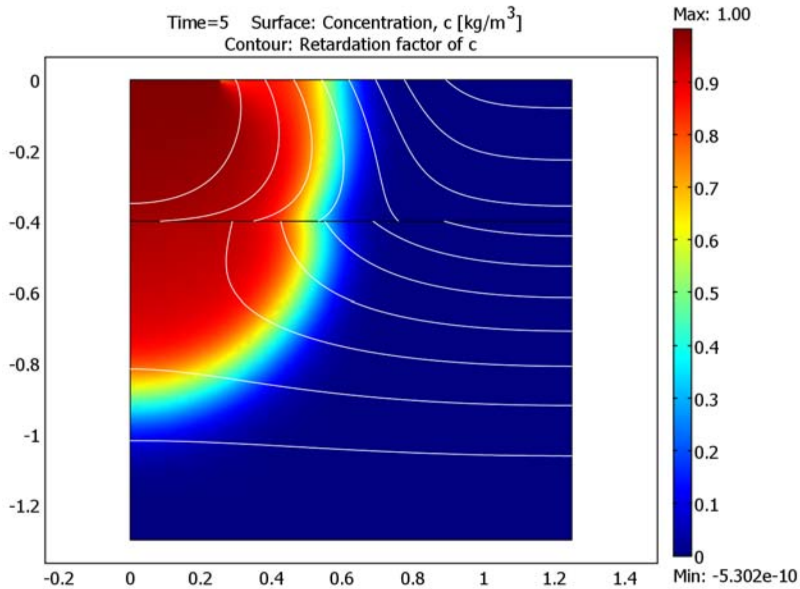


Figure 4-15: Solution for dissolved concentrations (surface plot) and retardation factor (contours) at 1 day.

Figure 4-16 shows an image of the retardation factor. For variably saturated solute transport, the retardation factor changes with time. As shown in this image, the process of sorption has the greatest potential to slow the contaminant where the soils are relatively dry for this example. In that the retardation coefficient here ranges from roughly 1.3 to 1.6, the solute moves at approximately the velocity of the groundwater.

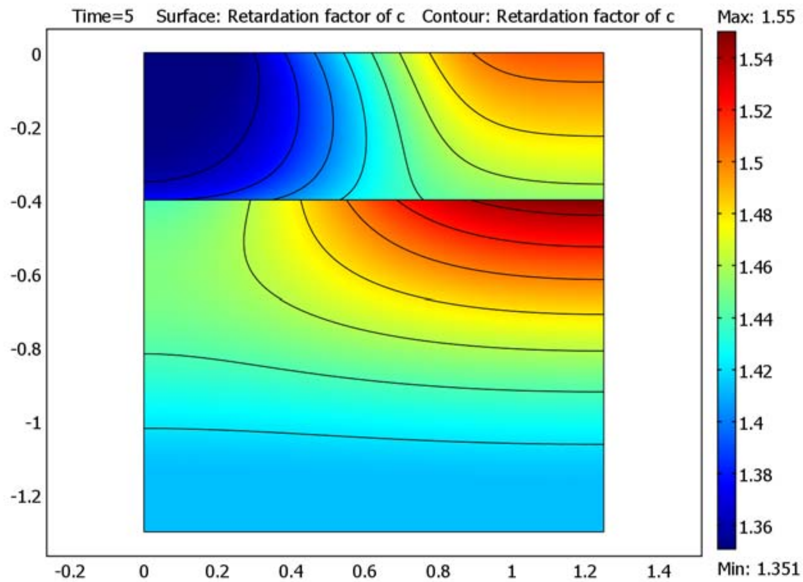


Figure 4-16: Snapshot of the retardation factor (surface and contours).

References

1. J. Simunek, T. Vogel and M.Th. van Genuchten, *The SWMS_2D code for simulating water flow and solute transport in two-dimensional variably saturated media*, ver. 1.1., Research Report No. 132, U.S. Salinity Laboratory, USDA, 1994.

2. J. Simunek, M. Senja, and M.Th. van Genuchten, *The HYDRUS-2D software package for simulating the two-dimensional movement of water, heat, and multiple solutes in variably-saturated media*, ver. 2.0, International Ground Water Modeling Center IGWMC-TPS 53, Colorado School of Mines, 1999.

3. M.Th. van Genuchten, "A closed-form equation for predicting the hydraulic of conductivity of unsaturated soils," *Soil Sci. Soc. Am. J.*, vol. 44, pp. 892–898, 1980.

4. R.H. Brooks and A.T. Corey, "Properties of porous media affecting fluid flow," *J. Irrig. Drainage Div.*, ASCE Proc. 72(IR2), pp. 61–88, 1966.

5. J. Bear, J, *Hydraulics of Groundwater*, McGraw-Hill Inc., 1978.

Model Library path: `Earth_Science_Module/Solute_Transport/sorbing_solute`

Modeling Using the Graphical User Interface

The following steps walk you through this model, setting up both the Richards' Equation application mode and the Solute Transport application mode. You can easily bypass a few of the details by using the example "Interpolation for Unsaturated Flow" on page 115 and adding to it the transport application. To do so, open the model file, add the Solute Transport application mode as described in the following description and then skip to the section "Physics—Solute Transport".

To start from scratch, first add the Richards' Equation application mode:

MODEL NAVIGATOR

1. Open the **Model Navigator**, and from the **Space dimension** list select **Axial symmetry (2D)**.
2. In the list of application modes select **Earth Science Module>Fluid Flow>Richards' Equation>Pressure head analysis>Transient analysis**.
3. Click the **Multiphysics** button, then click **Add**.
4. In the list of application modes select **Earth Science Module>Solute Transport>Variably Saturated Porous Media>Transient analysis**. Click **Add**.
5. Click **OK**.

CONSTANTS

First define some constants. Open the **Physics>Constants** list and define the following list (the descriptions are optional). When done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
phiL	0.05[1/s]	Decay rate in liquid
phiP	0.01[1/s]	Decay rate on solid
rhob	1400[kg/m^3]	Bulk density
kp	0.0001[m^3/kg]	Partition coefficient

APPLICATION SCALAR VARIABLES

To set the vertical direction and gravitational constant in the model, go to the **Physics** menu and open the **Scalar Variables** dialog box**.** Make the following modifications to the defaults. Here you convert from seconds to days and square the quantity because you are dealing with acceleration. Then click **OK**.

NAME	EXPRESSION
`D_esvr`	`z`
`g_esvr`	`9.82*86400*86400`

GEOMETRY MODELING

You create the geometry by drawing one rectangle and adding two lines.

1 Select the menu item **Draw>Specify Objects>Rectangle**. Specify the following settings, then click **OK**.

PARAMETER	EXPRESSION
width	`1.25`
height	`1.3`
r	`0`
z	`-1.3`

2 Go to the Main toolbar and click the **Zoom Extents** button.

3 Again select **Draw>Specify Objects>Rectangle**. Specify the following settings, then click **OK**.

PARAMETER	EXPRESSION
width	`1.25`
height	`0.4`
r	`0`
z	`-0.4`

4 Select the menu item **Draw>Specify Objects>Line**. In the **r** edit field enter `0 0.25`, and in the **z** edit field enter `0 0`. Click **OK**.

PHYSICS—RICHARDS' EQUATION

Subdomain Settings—Richards' Equation

1 To define the setting for the flow application mode, go to the **Multiphysics** menu and choose **Richards' Equation (esvr)**.

2 Choose **Physics>Subdomain Settings** and click the **Coefficients** tab. Enter the following settings, then click **Apply**.

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
Constitutive relation	van Genuchten	van Genuchten
θ_s	0.339	0.399
θ_r	0	0.0001
Storage term	User defined	User defined
S	0.339	0.399
K_S	0.454	0.298
ρ_f	1000	1000

3 Click the **van Genuchten** tab and make the following changes:

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
α	1.39	1.74
n	1.6	1.38
l	0.5	0.5

4 Click the **Init** tab. Select both subdomains simultaneously using the Ctrl key, then in the edit field enter this expression:

SETTING	SUBDOMAINS 1, 2
H_{P0}	`-(z+1.2)*(z<-0.4)+(-(z+1.2)-0.2*(z+0.4))*(-0.4<=z)`

5 Click **OK**.

Boundary Conditions—Richards' Equation

From the **Physics** menu choose **Boundary Settings** and make these settings; when done, click **OK**.

BOUNDARIES	BOUNDARY CONDITION	VARIABLE	EXPRESSION
1, 3, 4, 6–8	Zero flux/Symmetry		
2	Inward flux	N_0	-0.454/100
5		R_b	1*(t>=0)
5	Mixed	H_{pb}	0.01*(t>=0)
5		D_b	D_esvr*(t>=0)

PHYSICS—SOLUTE TRANSPORT

Enter the setting in the transport application mode by going to the **Multiphysics** menu and selecting **Solute Transport (esst)**.

Subdomain Settings—Solute Transport

Set up the material properties.

1 Choose **Physics>Subdomain Settings**. On the **Flow and Media** page enter these settings.

SETTINGS	SUBDOMAINS 1, 2
θ	`theta_esvr`
θ_s	`thetas_esvr`
u	`u_esvr`
v	`v_esvr`

Click **Apply**.

2 Click the **Liquid** tab and make the following changes. Click **Apply** after you have finished changing the values for each subdomain.

SETTINGS	SUBDOMAINS 1, 2
α_1	`0.005`
α_2	`0.001`
D_{mL}	`0.00374`
R_L	`-phiL*theta_esvr*c`
S_o	`-c*C_esvr*pt`

3 Click the **Solid** tab and make the following changes. Click **Apply** after you have finished changing the values for each subdomain.

TERM	SUBDOMAINS 1, 2
ρ_b	`rhob`
K_P	`kp`
R_P	`phiP*kp*rhob*c`

4 Click **OK**.

Boundary Conditions—Solute Transport

1 From the **Physics** menu choose **Boundary Settings** and make these settings; when done, click **OK**.

BOUNDARY	CONDITION	VARIABLE	EXPRESSION
1, 3, 6	No flux/Symmetry		
2, 7, 8	Advective flux		
5	Flux	N_0	`1e6[m/s]*(-c+1)*(t>=0)`

The factor 10^6 is a large number that implements the stiff-spring condition (see "Implementation—Stiff-Spring Condition" on page 252) and should not be interpreted as a physical velocity. The added unit makes the flux expression dimensionally correct.

MESH GENERATION

1 Go to the menu item **Mesh>Free Mesh Parameters**.

2 Click the **Boundary** tab. Select the upper surface and the break between the two soil layers (Boundaries 4, 5, and 6). In the **Maximum element size** edit field enter `0.02`.

3 Click **OK**.

4 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

1 Select the menu item **Solve>Solver Parameters**. In the **Solver** list choose **Time dependent** if it is not already selected.

2 In the **Times** edit field enter `-0.1,0,logspace(-3,-1,21),0.1:0.1:1,2:1:10`. It gives you 31 logarithmically spaced inputs from 0.001 to 0.1 day; 0.1-day increments through Day 1; and 1-day increments until Day 10.

3 Click the **Advanced** tab. Set the **Type of scaling** to **Manual**. Enter `p 1e10 c 1` in the **Manual scaling** edit field. Click **OK**.

4 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the plot in Figure 4-12, follow these steps:

1 Select the menu item **Postprocessing>Plot Parameters**.

2 On the **General** page go to the **Plot type** area and select the **Surface**, **Contour**, and **Arrow** check boxes. In the **Solution at time** list select **0.3**.

3 Click the **Surface** tab, and in the **Expression** edit field type `Se_esvr`, which stands for the effective saturation, Se, calculated with this application mode, named esvr.

4 Click the **Contour** tab, and in the list of **Predefined quantities** select **Pressure head (esvR)**. Go to the **Contour levels** area. Select the option button associated with **Vector with isolevels**, then in the edit field enter `-2:0.1:2`. In the **Contour color** area click the **Uniform color** option button, click the **Color** button, and change the color to white, and click **OK**. Clear the **Color scale** check box.

5 Click the **Arrow** tab, and in the list of **Predefined quantities** select **Richards' Equation (esvr)>Velocity field**. Go to the **Arrow parameters** area and click the **Color** button. Choose white as the color, then click **OK**. Clear the **Auto** check box and change the **Scale factor** to `0.5`. Click **Apply**.

To generate Figure 4-13 on page 255, select the menu item **Postprocessing>Plot Parameters** and in the **Solution at time** list select **1**. Click **OK**.

To generate the plot in Figure 4-14 on page 256, continue with these steps:

1 Select the menu item **Postprocessing>Plot Parameters**.

2 In the **Plot type** area clear the **Arrow** check box. In the **Solution at time** list choose **0.3**.

3 Click the **Surface** tab, and in the list of **Predefined quantities** select **Concentration, c**.

4 Click the **Contour** tab, and from the list of **Predefined quantities** select **Solute Transport (esst)>Retardation factor of c**. Go to the **Contour levels** area, select the **Vector with isolevels** option button, and in the associated edit field enter `-2:0.1:2`. In the **Contour color** area select the **Uniform color** option button. Click the **Color** button, change the color to black, and click **OK**.

5 Click **Apply**, but leave this dialog box open.

To generate Figure 4-15 on page 257, return to the **General** tab, and in the **Solution at time** list select **1**. Click **OK**.

1 To generate Figure 4-16 on page 258, select the menu item **Postprocessing>Plot Parameters**. In the **Plot type** area clear the **Contour** check box. In the **Solution at time** list select **0.2**. Click **Apply.**

2 Click the **Surface** tab, and in the list of **Predefined quantities** select **Solute Transport (esst)>Retardation factor of c**. Click **OK**.

SAVING THE MODEL

This completes the model. In the following sections you add new equations and terms. Save the current model by choosing **File>Save As** and entering a file name. Click **OK**.

Pesticide Transport and Reaction in Soil

Introduction

Aldicarb is a commercial pesticide, used on a variety of crops, including cotton, sugar beet, citrus fruits, potatoes, and beans. The general population may be exposed to aldicarb primarily through the ingestion of contaminated water and foods.

This example looks at the degradation kinetics of aldicarb and its toxic by-products, investigating both the degradation time-scale as well as the spatial concentration distribution of toxic components. In the first model the chemicals are contained in a water pond, treated as a perfectly mixed system. The second model tracks the detailed distribution of chemicals in soil as the pesticide leaches out of the pond and is transported in water through the ground.

The reaction kinetics describing the degradation pathways of aldicarb is exported to the Solute Transport application mode of the Earth Science Module. In COMSOL Multiphysics the solute transport is coupled to fluid flow as described by Richards' equation.

Note: This model requires the COMSOL Reaction Engineering Lab and the Earth Science Module.

Model Definition

Aldicarb degrades by transformation to the corresponding sulfoxide and the sulfone (both of which are toxic), and is detoxified by hydrolysis to oximes and nitriles. The chain of reactions is illustrated in Figure 4-17. The toxicity of a chemical species is indicated by its LD_{50} value, signifying the dose (mg/kg) lethal to half of a test population of rats. As indicated, both the sulfoxide and solfone analogues of aldicarb are also relatively toxic.

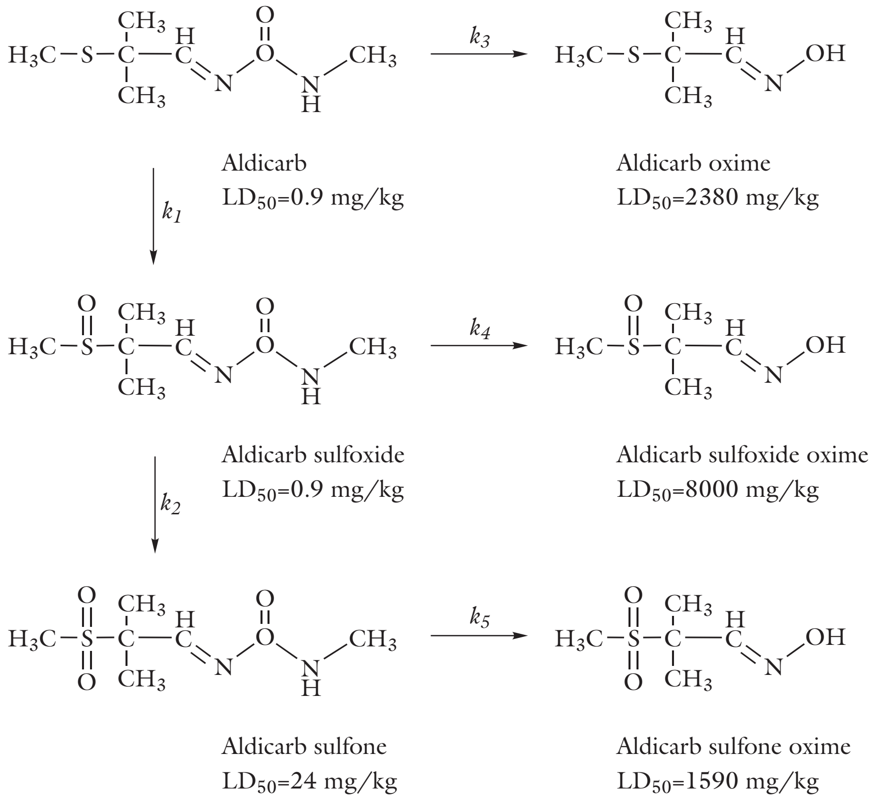


Figure 4-17: Reaction pathways of aldicarb degradation.

Each of the j unimolecular reactions outlined above have rate expressions of the form:

$$r_j = k_j c_i$$

Note that in this example the concentration unit is kg/m^3 and the rate constants are expressed in 1/day.

PERFECTLY MIXED SYSTEM

The first model solves for the decomposition kinetics of aldicarb occurring in a water pond. The pond is treated as a closed and perfectly mixed system. The reaction mechanism illustrated in Figure 4-17 translates into the following mass balance equations:

- For aldicarb (a)

$$\frac{dc_a}{dt} = -r_1 - r_3$$

- For aldicarb sulfoxide (asx)

$$\frac{dc_{\text{asx}}}{dt} = r_1 - r_2 - r_4$$

- For aldicarb sulfone (asn)

$$\frac{dc_{\text{asn}}}{dt} = r_2 - r_5$$

- For aldicarb oxime (ao)

$$\frac{dc_{\text{ao}}}{dt} = r_3$$

- For aldicarb sulfoxide oxime (asxo)

$$\frac{dc_{\text{asxo}}}{dt} = r_4$$

- For aldicarb sulfone oxime (asno)

$$\frac{dc_{\text{asno}}}{dt} = r_5$$

Solving this set of coupled ODEs outlined above provides information on the time scale of the degradation processes.

SPACE- AND TIME-DEPENDENT SYSTEM

In a more detailed model, you assume that aldicarb moves from the pond into relatively dry soil. In the soil, the aldicarb decomposes according to the mechanism illustrated in Figure 4-17. In addition, the pesticide and its decay products are transported by advection, dispersion, sorption, and volatilization.

Geometry

Water is ponded by a ring sitting on the ground. The soil is layered and rests on rocks. Water moves through the bottom of the ring into the soil. The water level in the ring is known. There is no flow through the vertical walls or the surface outside of the ring.

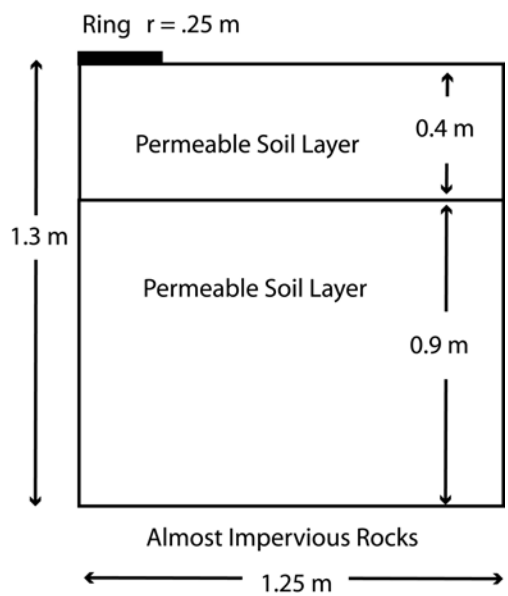


Figure 4-18: Geometry of the infiltration ring and soil column.

Aldicarb moves with water from the pond into the soil at a constant concentration. In the soil, the chemicals react and also sorb onto soil particles. Aldicarb and the aldicarb sulfone volatilize to the atmosphere. The sorption, biodegradation, and volatilization proceed in linear proportion to the aqueous concentrations. The soil is initially pristine with zero concentration of the involved chemicals. At the ground surface outside the ring, there is volatilization to the atmosphere for c_{a} and c_{asn}. The vertical axis is a line of symmetry. The other boundaries are posed such that the solutes can freely leave the soil column with the fluid flow. You can model the problem with 2D axisymmetry and track the solute transport for 10 days.

Fluid Flow

Richards' equation governs the saturated-unsaturated flow of water in soil (Ref. 1) and is implemented in the Richards' equation application mode:

$$[C + \mathrm{Se}S]\frac{\partial H_p}{\partial t} + \nabla \cdot [-K_s k_r \nabla(H_p + D)] = Q_s$$

Here, C denotes specific moisture capacity (m^{-1}), Se is the effective saturation of the soil, S is a storage coefficient (m^{-1}), H_p represents the dependent variable pressure head (m), t is time (d), K equals the hydraulic conductivity function (m/d), D is the coordinate representing vertical elevation (for example, x, y, or z), and Q_s is a fluid source defined by volumetric flow rate per unit volume of soil (d^{-1}). In this problem, $S = \theta_s - \theta_r$, where θ_s and θ_r denote the volume fraction of fluid at saturation and after drainage, respectively.

You can find more detail on the Richards' Equation application mode in the Earth Science Module User's Guide.

Mass Transport

The governing equation for solute transport describes advection and dispersion of a sorbing, volatilizing, and decaying solute in variably saturated soil.

$$\left[\theta + \rho_b\frac{\partial c_p}{\partial c} + a_v\frac{\partial c_G}{\partial c}\right]\frac{\partial c}{\partial t} + \left[(1 - k_G)c\frac{\partial \theta}{\partial t}\right] + \nabla \cdot [-\theta \mathrm{D}_{LG}\nabla c + \mathbf{u}c] = R_L + R_P + R_G + S_c \tag{4-2}$$

Equation 4-2 is implemented in the Solute Transport application mode. The first bracketed term explains the change in solute mass per volume per time for the liquid-, solid-, and air-phase concentrations. The second term explains the changes in storage because the water content in the soil varies in time. The third bracketed expression represents the overall solute flux due to liquid dispersion, diffusion (liquid and air), and advection with moving water. The right side explains reactions and generalized sources.

Solute spreading now includes mechanical dispersion in water plus molecular diffusion for water and air. These three processes appear in the liquid-gas dispersion tensor, whose entries are

$$\theta D_{LGii} = \alpha_1\frac{u_i^2}{|\mathbf{u}|} + \alpha_2\frac{u_j^2}{|\mathbf{u}|} + \theta D_m \tau_L + a_v D_G k_G \tau_G \tag{4-3}$$

$$\theta D_{LGij} = \theta D_{LGji} = (\alpha_1 - \alpha_2)\frac{u_i u_j}{|\mathbf{u}|} \tag{4-4}$$

In this equation, D_{LGii} are the principal components of the liquid-gas dispersion tensor; D_{LGij} and D_{LGji} are the cross terms; α is the dispersivity (m) where the subscripts $_1$ and $_2$ denote longitudinal and transverse flow, respectively. D_m and D_G (m^2/d) are molecular diffusion, while τ_L and τ_G give the tortuosity factors for liquid (water) and gas (air), respectively.

The three solutes—aldicarb, aldicarb sulfoxide, and aldicarb sulfone—have different decay terms, R_{Li}, partition coefficients, k_{Pi}, and volatilization constants, k_{Gi}. All of the solutes attach to soil particles. Two of the solutes volatilize; sulfoxide does not.

Results

First, review the results of the perfectly mixed reactor model, solved in the Reaction Engineering Lab.

Figure 4-19 shows the concentration profile of aldicarb and all of its decay products. Only small amounts of aldicarb remain after 10 days. Figure 4-20 shows concentration transients of the most toxic species aldicarb, aldicarb sulfoxide, and aldicarb sulfone, as well as the sum of these three components (see Figure 4-17 for LD_{50} values). Considering the summed contributions, contamination levels clearly remain high even after several months.

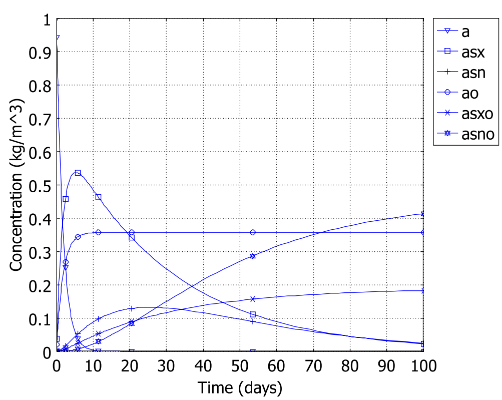


Figure 4-19: Concentration profiles (kg/m^3) as reactions occur during a 100 day time period.

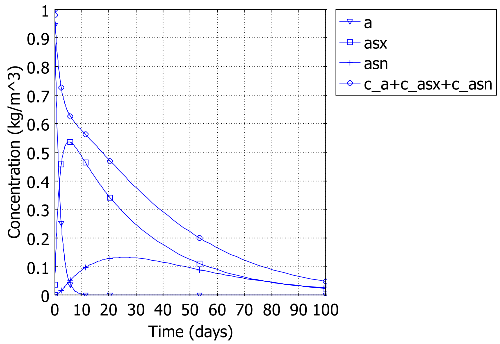


Figure 4-20: Concentration transients of the most toxic species, aldicarb (c_a), aldicarb sulfoxide (c_asx), and aldicarb sulfone (c_asn).

Results shown below come from the space and time-dependent model set up and solved in COMSOL Multiphysics.

Figure 4-21 shows the fluid flow in soil after 0.3 days (left) and 1.0 days (right). The plots illustrate the wetting of the soil with time. As indicated by the arrows, the fluid velocities are relatively high beneath the ponded water.

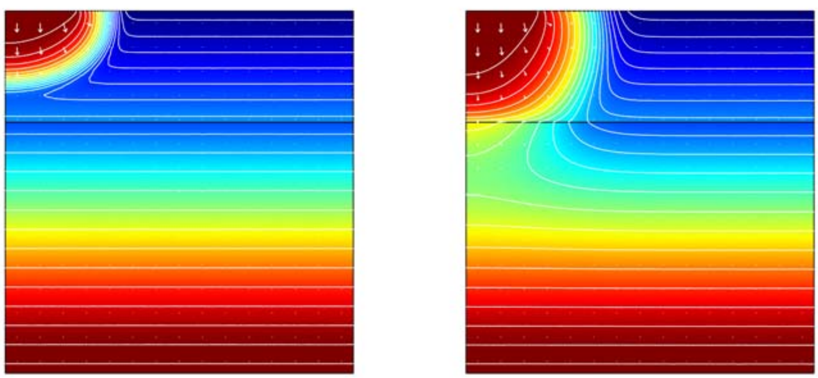


Figure 4-21: The effective saturation (surface plot), pressure head (contours), and flow velocity (arrows) in a variably saturated soil after 0.3 days (left) and 1 day (right).

Figure 4-22 through Figure 4-24 show the concentration distribution of aldicarb and the equally toxic aldicarb sulfoxide, after 1, 5, and 10 days of infiltration. Consistent with the evolving flow field, the main direction of transport is in the vertical direction.

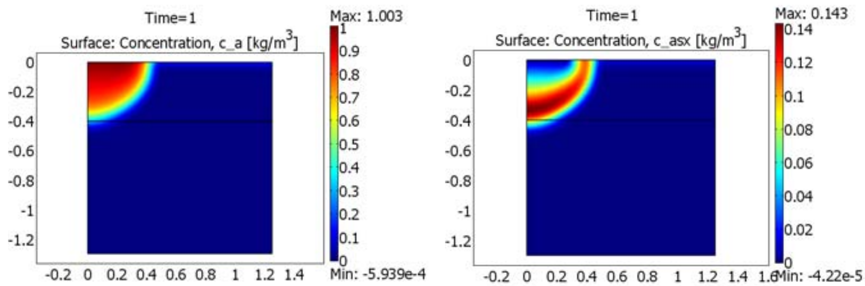


Figure 4-22: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 1 day.

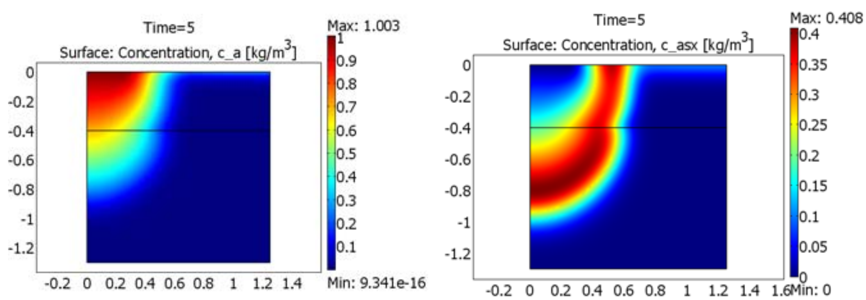


Figure 4-23: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 5 days.

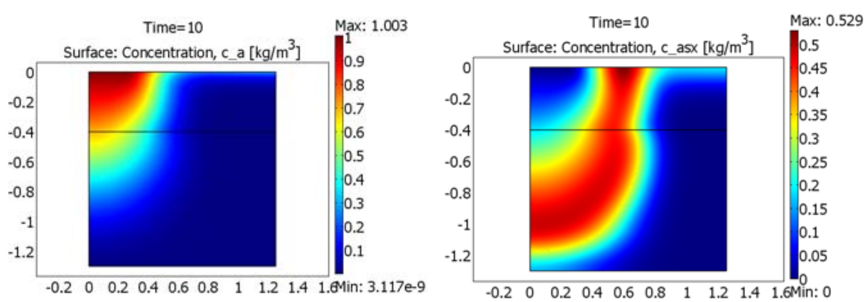


Figure 4-24: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 10 days.

The distribution of aldicarb has clearly reached steady-state conditions after 10 days. This time frame was also predicted by the ideal reactor model. Results also show that the soil contamination is rather local with respect to the aldicarb source. The aldicarb sulfoxide, on the other hand, can be expected to affect a considerably larger soil volume for a significantly longer time.

References

1. J. Bear, J, *Hydraulics of Groundwater,* McGraw-Hill Inc., 1978.

2. M.Th. van Genuchten, "A closed-form equation for predicting the hydraulic of conductivity of unsaturated soils," *Soil Sci. Soc. Am. J.*, vol. 44, pp. 892–898, 1980.

Model Library path: `Earth_Science_Module/Solute_Transport/pesticide_transport`

Modeling Using the COMSOL Reaction Engineering Lab

MODEL NAVIGATOR

1. Start COMSOL Reaction Engineering Lab.
2. Click **New** in the **Model Navigator**.

OPTIONS AND SETTINGS

1. Click the **Model Settings** button on the Main toolbar.
2. Select the **Liquid** from the **Reacting fluid** list.
3. Select the **Calculate thermodynamic properties** check box.
4. Select the **Calculate species transport properties** check box.
5. Click **Close**.

REACTIONS INTERFACE

1. Click the **Reaction Settings** button on the Main toolbar.
2. Make sure the **Reactions** page is active. Create five entries in the **Reaction selection** list by clicking the **New** button

3 Enter the following reaction formulas by first selecting the appropriate row in the **Reaction selection** list and then entering the corresponding text in the **Formula** edit field.

REACTION ID #	REACTION FORMULA
1	`a=>asx`
2	`asx=>asn`
3	`a=>ao`
4	`asx=>asxo`
5	`asn=>asno`

4 Type in the following rate constants by first selecting the appropriate row in the **Reaction selection** list and then entering the corresponding value in the $\mathbf{k^f}$ edit field.

REACTION ID #	FORWARD RATE CONSTANT
1	`0.36`
2	`0.024`
3	`0.2`
4	`0.01`
5	`0.0524`

SPECIES INTERFACE

1 Click the **Species** tab.

2 Select the entry **a** from the **Species selection** list and type `1` in the $\mathbf{c_0}$ edit field.

3 Go to the **Transport** page.

4 Select all entries in the **Species selection** list by pressing Ctrl+A and clicking the list.

5 Click the **Specify diffusivity** check box and type `0.00374` in the **Diffusivity** edit field.

6 Click **Close**.

COMPUTING THE SOLUTION

1 Click the **Solver Parameters** button on the Main toolbar.

2 Go to the **Times** edit field and enter `100`. Note that the time unit in this example is days.

3 Click **OK**.

4 Compute the solution by clicking the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The concentration transients of all species are plotted by default as shown in Figure 4-19. Reproduce Figure 4-20 with the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 Remove the entries ao, asxo, asno from the **Quantities to plot** list by selecting them and clicking the **<** button.

3 Type `c_a+c_asx+c_asn` in the **Expression** edit field and click the associated **>** button.

4 Click **OK**.

Now, move on to export the reaction model to COMSOL Multiphysics and solve the time and space-dependent transport and reaction problem.

SPECIES INTERFACE

This model focuses on the concentration of the highly toxic species aldicarb (a), aldicarb sulfoxide (asx), and aldicarb sulfone (asn). Therefore, you can disregard the mass balances for the hydrogenolysis products (ao, asxo, and asno). Before exporting the reaction model you therefore deactivate these species.

1 Click the **Reaction Settings** button on the Main toolbar.

2 Click the **Species** page.

3 Select **ao** from the **Species selection** list and deactivate the species by clearing the check box immediately to the left of the species name.

4 In the same way, deactivate the species asxo and asno.

5 Click **Close**.

EXPORT SETTINGS

1 Click the **Export to COMSOL Multiphysics** button on the Main toolbar.

2 Select **Axial symmetry (2D)** from the **Space dimension** list, then click **OK**.

3 The **Export to COMSOL Multiphysics** dialog box appears.

4 Go to the **Export mass balance** area, and in the **Application mode** list select **Solute Transport: New**.

5 In the **Group name** edit field type `reactions`.

6 Move to the **Export energy balance** area and clear the check box in the upper left corner.

7 Go to the **Export momentum balance** area and clear the check box in the upper left corner.

8 Click the **Export** button at the bottom of the dialog box.

Modeling Using COMSOL Multiphysics

Click the **COMSOL Multiphysics** window.

1 Select the menu item **Multiphysics>Model Navigator**.

   Note how the model already contains the application mode **Solute Transport**, created by the export from Reaction Engineering Lab.

2 In the list of application modes select **Earth Science Module>Fluid Flow>Richards' Equation>Pressure head analysis>Transient analysis**.

3 Click the **Add** button.

4 Click **OK**.

APPLICATION SCALAR VARIABLES

To set the vertical direction and gravitational constant in the model, go to the **Physics** menu and choose **Scalar Variables**. Make the following modifications to the defaults. Here you convert from seconds to days and square the quantity because you are dealing with acceleration. When done, click **OK**.

NAME	EXPRESSION
g_esvr	`9.82*86400*86400`
D_esvr	`z`

GEOMETRY MODELING

You create the geometry by drawing two rectangles and adding one line.

1 Select the menu item **Draw>Specify Objects>Rectangle**. Specify the following settings, then click **OK**.

PARAMETER	EXPRESSION
Width	`1.25`
Height	`1.3`
r	`0`
z	`-1.3`

2 Go to the Main toolbar and click the **Zoom Extents** button.

3 Again select **Draw>Specify Objects>Rectangle**. Specify the following settings, then click **OK**.

PARAMETER	EXPRESSION
Width	`1.25`
Height	`0.4`
r	`0`
z	`-0.4`

4 Select the menu item **Draw>Specify Objects>Line**. In the **r** edit field enter `0 0.25`, and in the **z** edit field enter `0 0`. Click **OK**.

PHYSICS—SOLUTE TRANSPORT

1 Choose **Multiphysics>Solute Transport (esst)**.

2 Select the menu item **Physics>Properties**.

3 Select **Liquid/Solid/Gas** from the **Material** drop down list, then click **OK**. You change the default settings as a three phase system is being modeled.

4 Select the menu item **Physics>Subdomain Settings**. In the **Subdomain selection** list simultaneously select Subdomains 1 and 2 by pressing the Ctrl key.

5 From the **Group** list, select **reactions**.

6 Go to the **Flow and Media** page, enter the following settings.

PROPERTY	VALUE
θ	`theta_esvr`
θ_s	`thetas_esvr`
u	`u_esvr`
v	`v_esvr`

This couples the solute transport to the flow calculated by the Richards' Equation (esvr) application mode.

7 Set the **Time change in liquid volume fraction** to **Time change in pressure head** and enter the following.

PROPERTY	VALUE
C	`C_esvr`
$\partial H_p/\partial t$	`pt`

8 Click the **Liquid** page. In the list of subdomains, simultaneously select **1** and **2** by pressing Ctrl. Make the changes in the following table, and note that you can copy and paste in the edit fields.

TERM	C_A	C_ASX	C_ASN
α_l	0.005	0.005	0.005
α_2	0.0001	0.0001	0.0001

Note also that the $\mathbf{D_{mL}}$ and $\mathbf{R_L}$ edit fields have been filled out automatically as a result of the export from COMSOL Reaction Engineering Lab.

9 Click the **Solid** page. Select both Subdomain 1 and 2, then make the following changes:

TERM	C_A	C_ASX	C_ASN
ρ_b	1300	1300	1300
K_P	0.0001	0.00005	0.0002

10 Click the **Gas** page, select Subdomains 1 and 2, then make the following changes:

TERM	C_A	C_ASX	C_ASN
k_G	1.33e-7	0	1.33e-3
D_{mG}	0.432	0.432	0.432

11 Go to the **Init** page and type `0` in the $\mathbf{c\_a(t_0)}$ edit field.

12 Click **OK**.

Boundary Conditions—Solute Transport

1 From the **Physics** menu choose **Boundary Settings**.

2 Verify that you are on the **c_a** page, then enter the following settings:

BOUNDARY	CONDITION	VARIABLE	VALUE
1, 3	Axial symmetry		
2, 7, 8	Advective flux		
5	Flux	N_0	`1e6*(1-c_a)*(t>=0)`
6	No flow boundary volatilization	d	0.005

3 Click the **c_asx** page, then enter the following settings:

BOUNDARY	CONDITION	VARIABLE	VALUE
1, 3,	Axial symmetry		
6	No flux/Symmetry		
2, 7, 8	Advective flux		
5	Concentration	c_asx_0	0

4 Click the **c_asn** page, then enter the following settings:

BOUNDARY	CONDITION	VARIABLE	VALUE
1, 3	Axial symmetry		
2, 7, 8	Advective flux		
5	Concentration	c_asn_0	0
6	No flow boundary volatilization	d	0.005

5 Click **OK**.

PHYSICS—RICHARDS' EQUATION

Subdomain Settings—Richards' Equation

1 Go to the **Multiphysics** menu and choose **Richards' Equation (esvr)**.

2 Select the menu item **Physics>Subdomain Settings** and click the **Coefficients** page. Enter the following settings, then click **Apply**.

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
Constitutive relation	van Genuchten	van Genuchten
θ_s	0.339	0.399
θ_r	0	0.0001
Storage term	User defined	User defined
S	0.339	0.399
K_S	0.454	0.298
ρ_f	1000	1000

3 Click the **van Genuchten** page and make the following changes:

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
α	1.39	1.74

SETTINGS	SUBDOMAIN 1	SUBDOMAIN 2
n	1.6	1.38
l	0.5	0.5

4 Click the **Init** page. Select both subdomains simultaneously using the Ctrl key, then in the edit field enter this expression:

SETTING	SUBDOMAINS 1 AND 2
$H_P(t_0)$	`-(z+1.2)*(z<-0.4)+(-(z+1.2)-0.2*(z+0.4))*(-0.4<=z)`

5 Click **OK**.

Boundary Conditions—Richards' Equation

1 From the **Physics** menu choose **Boundary Settings** and make these settings:

BOUNDARY	BOUNDARY CONDITION	VARIABLE	EXPRESSION
1, 3	Axial symmetry		
6–8	Zero flux/Symmetry		
2	Inward flux	N_0	`-0.454/100`
5	Mixed	R_b	`1*(t>=0)`
5		H_{pb}	`0.01*(t>=0)`
5		D_b	`D_esvr*(t>=0)`

2 Click **OK**.

MESH GENERATION

1 Go to the menu item **Mesh>Free Mesh Parameters**.

2 Click the **Boundary** page. Select the upper surface and the break between the two soil layers (Boundaries 4, 5, and 6). In the **Maximum element size** edit field enter `0.02`.

3 Click **OK**.

4 Click the **Initialize Mesh** button on the Main toolbar.

COMPUTING THE SOLUTION

This model has many degrees of freedom and is also nonlinear. It requires roughly an hour to solve on a fast computer.

1 Choose **Solve>Solver Parameters**.

2 In the **Solver** list choose **Time dependent** if it is not already selected.

3 In the **Times** edit field enter `-0.1,0,logspace(-3,-1,21),0.1:0.1:1,2:1:10`. It gives you 31 logarithmically spaced inputs from 0.001 to 0.1 day; 0.1-day increments through Day 1; and 1-day increments until Day 10.

4 Click the **Advanced** page.

5 Change the **Type of scaling** to **Manual**.

6 Type `p 1e10 c_a 1 c_asx 1 c_asn 1` in the **Manual scaling** edit field.

7 Click **OK**.

8 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To plot the flow solution in Figure 4-21, follow these steps.

1 Select the menu item **Postprocessing>Plot Parameters**.

2 On the **General** page go to the **Plot type** area and select the **Surface**, **Contour**, and **Arrow** check boxes.

3 From the **Solution at time** list choose **0.3**.

4 Click the **Surface** page, and in the **Expression** edit field enter `Se_esvr`.

5 Click the **Contour** page, and in the **Predefined quantities** list choose **Richards' Equation (esvr)>Pressure head**.

6 In the **Contour color** area, click the **Uniform color** option button. Click the **Color** button, change the color to white, and click **OK**.

7 Click **Apply**.

8 Click the **Arrow** page.

9 From the list of **Predefined quantities** select **Richards' Equation (esvr)>Velocity field**.

10 Click the **Color** button, choose white as the desired color, then click **OK**.

11 Clear the **Auto** check box, and in the **Scale factor** edit field enter `0.5`.

12 Click **Apply**.

13 To generate the solution after 1 day, go to the **General** page and select 1 from the **Solution at time** list, and then click **OK**.

To generate the plots in Figure 4-22 through Figure 4-24, continue with these steps:

1 Select the menu item **Postprocessing>Plot Parameters**.

2 On the **General** page, clear the **Arrow** and **Contour** check boxes.

3 Click the **Surface** page, then type `c_a` in the **Expression** edit field.

4 Click **Apply**.

5 To generate the solution after 5 days and 10 days, go to the **General** page and select the corresponding entries from the **Solution at time** list, and click **Apply**.

6 To generate plots for the aldicarb sulfoxide concentrations, click the **Surface** page, type `c_asx` in the **Expression** edit field, then click **Apply**.

5

Heat Transfer Models

The models in this chapter demonstrate phase change, buoyancy flow, and free convection in porous media.

Buoyancy Flow in Free Fluids

This example follows the benchmark buoyancy flow posed by de Vahl Davis (Ref. 1) for free fluids. Buoyancy flow of free fluids is very important in earth sciences with temperature and concentration affecting density in fluids that move, for example, in pipes, along shorelines, and within lakes. Here the buoyancy flow results from density that varies with a temperature change. The COMSOL Multiphysics results match those from the published study (Ref. 1). The model was provided by John Kamel of the University of Notre Dame.

This example repeatedly solves a problem of buoyant flow in a square cavity. It thereby analyzes different temperature distributions and convective flow patterns from variations in, for example, fluid properties, cavity size, and temperature drops. The iterative process is tuned for a fast, efficient solution using nondimensional parameters and a Boussinesq term for the buoyant drive with the incompressible Navier-Stokes equation and the Convection and Conduction application modes. Another method to solve for the buoyant flow of free fluids in COMSOL Multiphysics using these application modes is simply to trigger the non-isothermal flow option, which enables modeling with a fully compressible Navier-Stokes flow law.

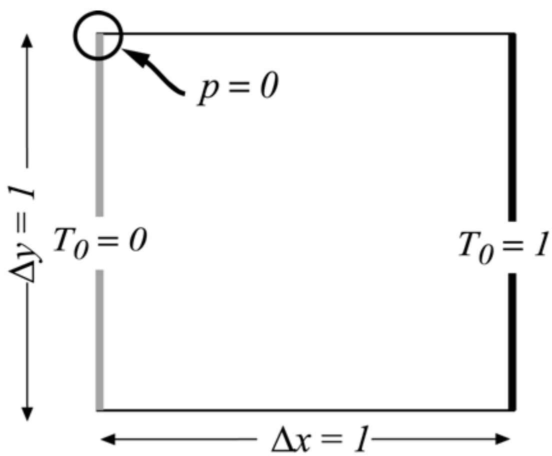


Figure 5-1: Domain geometry and boundary conditions for the heat balance in this example of buoyant flow in free fluids.

Model Definition

The previous figure illustrates the model geometry. The fluid fills a square cavity with impermeable walls so the fluid flows freely within it but does not exit from it. The right and left edges of the cavity are, respectively, the high and low temperature sources. The upper and lower boundaries are insulated. The temperature differential produces the density variation that drives the buoyant flow.

The flow and temperature application modes in this model are 2-way coupled. The Boussinesq term is a force defined on temperatures. The fluid velocities transport heat.

It is possible to formulate the Navier-Stokes equations with a Boussinesq buoyancy term on the right-hand side to account for the lifting force due to thermal expansion:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho_0\mathbf{g}\beta(T - T_0) \tag{5-1}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{5-2}$$

In these expressions, the dependent variables for flow are $\mathbf{u}$, a vector of directional velocities, and pressure, p. T represents temperature, T_0 is a reference temperature, $\mathbf{g}$ denotes gravity acceleration, ρ_0 gives the reference density, and β equals the thermal expansion coefficient.

The heat balance comes from the conduction-convection equation

$$C_L\mathbf{u}\nabla\cdot T - \nabla\cdot(K_{eq}\nabla T) = 0 \tag{5-3}$$

where K_{eq} denotes the thermal conductivity, and C_L is the volumetric heat capacity of the fluid (where $C_L = \rho_f C_p$, and C_p is the specific heat capacity).

The boundaries for the Navier-Stokes equations are impermeable, no-slip conditions. The no-slip condition results in zero velocity at the wall, with pressure within the domain remaining undefined. Because the lack of information about p makes it difficult for the problem to converge, you arbitrarily fix the pressure at a point using *point settings*.

The boundary conditions for Convection and Conduction application mode are the fixed high and low temperatures on the vertical walls, with insulation conditions elsewhere, as shown in Figure 5-1.

Implementation: Nondimensional Solutions with Iterative Solver

The model addresses a wide range of cavity sizes, fluid properties, and temperature drops using material properties set up with nondimensional Raleigh and Prandtl numbers. The Raleigh number, $\mathrm{Ra} = (g\beta T L^3)/(\eta\rho^{-1} K_{\mathrm{eq}}\, C_L^{-1})$, denotes the ratio of buoyant to viscous forces. Here L is the length of a side wall. The Prandtl number, $\mathrm{Pr} = (\eta\rho^{-1})/(K_{\mathrm{eq}}\, C_L^{-1})$, gives the ratio of kinematic viscosity to thermal diffusivity.

Setting $\rho = (\mathrm{Ra}\cdot\mathrm{Pr})^{0.5}$, $C_p = \mathrm{Pr}$, and $\eta = K_{\mathrm{eq}} = 1$ produces nondimensional p, $\mathbf{u}$, and T. The dimensional counterpart to the solution comes from the equations

$$x_i' = Lx_i, \quad t' = \frac{L}{U}t, \quad u_i' = \frac{u_i}{U}, \quad p' = \frac{p}{\rho_0 U^2}, \quad T' = \frac{T - T_h}{T_c - T_h}$$

where ' denotes dimensional quantities, and U is the magnitude of the velocity vector $\mathbf{u}$.

As Ra increases, viscous forces decrease in importance. You can examine a wide range of scenarios using the parametric solver and sequencing through different values of Ra but keeping Pr constant. At a high Ra, starting with a good initial condition and a well-tuned mesh becomes increasingly important. Because the parametric solver uses the previous solution as the initial condition for the next one, it fulfills the first of the two requirements. Then getting a well-tuned mesh is straightforward: simply set up the mesh for the most difficult problem to solve—the one with the highest value of Ra. To that end, the element size near the prescribed temperature boundaries corresponds to the thickness of the boundary layer when $\mathrm{Ra} = 10^6$.

Results

As noted earlier, this COMSOL Multiphysics example reproduces a benchmark buoyant flow problem reported in Ref. 1. The composite images in Figure 5-2 summarize temperatures (surface), velocity fields (arrows), and x-velocities (contours) for four Ra values. With the given definitions for the dimensionless variable, it follows that as Ra increases so does temperature. The results in the figure indicate how the vigor and complexity of the convection increase at higher values of Ra, as expected.These results are virtually identical to the benchmark solution except the COMSOL Multiphysics plots provide higher resolution than the images in the original publication.

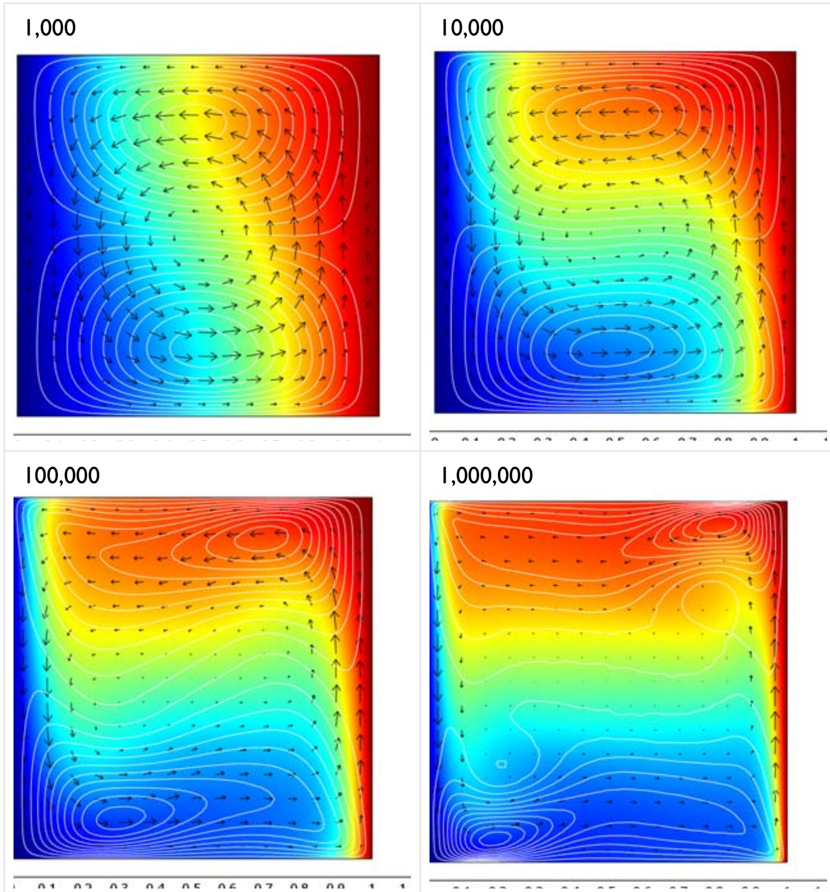


Figure 5-2: Dimensionless solution for buoyancy flow in a fluid-filled cavity at increasing Raleigh number: Temperature (surface plot), velocity field (arrows), and x-velocity (contours). These results from the COMSOL Multiphysics simulation and the published results (Ref. 1) are in excellent agreement.

Conclusions

The author built this model using predefined physics interfaces (application modes) from the Earth Science Module for the Navier-Stokes equations and heat transfer by convection and conduction. The modeling process lasted less than 1 hour including all the steps from geometry input to postprocessing results.

This approach represents the buoyant drive with a Boussinesq term, but you could also model it with the automated non-isothermal flow options provided with the Navier-Stokes application mode. Using the Boussinesq approach here, however, demonstrates a well-established method for conserving computational effort and still representing buoyant flow.

References

1. G. de Vahl Davis and I.P. Jones, “Natural convection in a square cavity—a comparison exercise,” *Int. J. Num. Meth. in Fluids*, vol. 3, pp. 227–248, 1983.

2. G. de Vahl Davis, “Natural convection of air in a square cavity: a bench mark numerical solution,” *Int. J. Num. Meth. in Fluids*, vol. 3, pp. 249–264, 1983.

Model Library path: `Earth_Science_Module/Heat_Transfer_Models/buoyance_free`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. Open the **Model Navigator**, click the **Multiphysics** button, and in the **Space dimension** list select **2D**.
2. In the list of application modes select **Earth Science Module>Fluid Flow>Incompressible Navier-Stokes Equations**. Click **Multiphysics**, then click **Add**.
3. In the list of application modes select **Earth Science Module>Heat Transfer>Convection and Conduction**, then click **Add**.
4. Click the **Application Mode Properties** button. In the **Material list** choose **Mobile Fluid**. Click **OK**.

OPTIONS AND SETTINGS

Select the menu item **Options>Expressions>Scalar Expressions**, then add the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
Ra	1e6	Raleigh number
Pr	0.71	Prandtl number
Th	1	High temperature
Tc	0	Low temperature

Because this is a nondimensional model, use no unit system:

1 From the **Physics** menu, choose **Model Settings**.

2 Select **None** from the **Base unit system** list in the **Model Settings** dialog box.

3 Click **OK**.

GEOMETRY MODELING

1 Go to the Draw toolbar on the left side of the user interface and select **Rectangle/Square**. Fill in the dialog box to create a square with corners at (0, 0) and (1, 1).

2 Click the **Zoom Extents** button on the Main toolbar to center the square within the viewing window.

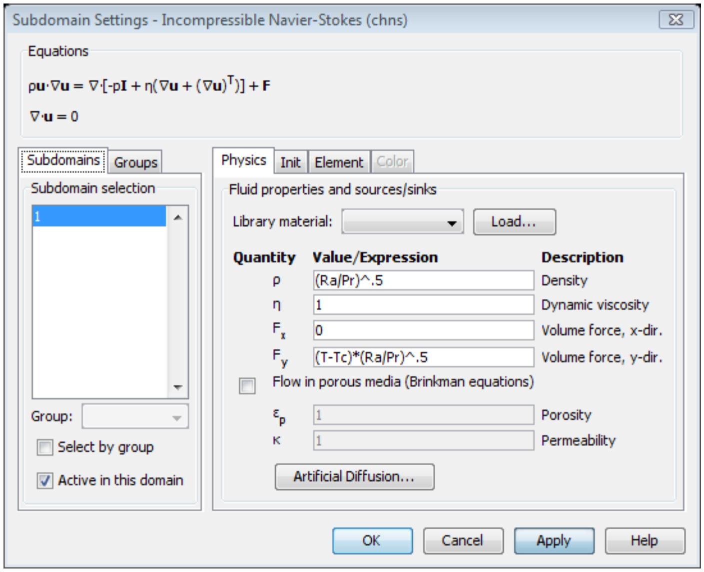
PHYSICS SETTINGS—FLOW

From the **Multiphysics** menu select **Incompressible Navier-Stokes equations (chns)**.

Subdomain Settings

Select the menu item **Physics>Subdomain Settings**, select Subdomain 1, then enter the following settings:

COEFFICIENT	EXPRESSION
ρ	(Ra/Pr)^.5
η	1
Fx	0
Fy	(T-Tc)*(Ra/Pr)^.5



Initial Conditions

Leave the initial conditions at their default values $u = v = p = 0$.

Boundary Conditions

The boundary conditions default to no-slip and need not to be altered.

Point Settings

Select the menu item **Physics>Point Settings**. Select Point 1, then select the **Point constraint** check box. Leave the $\mathbf{p_0}$ field at **0**. Click **OK**.

PHYSICS SETTINGS—HEAT TRANSFER

From the **Multiphysics** menu select **Convection and Conduction (eshcc)**.

Subdomain Settings

1. Select the menu item **Physics>Subdomain Settings**.
2. Go to the **Materials** page, and for the following parameters find the associated edit field and enter theses expressions:

VALUE	EXPRESSION
ρ_L	`(Ra/Pr)^.5`
Cp_L	`Pr`
K_L	`1`

3 Click the **Time/Convection** tab. Set the velocities in the heat transfer equation to the fluid velocities from the flow equation by entering these expressions for **u** and **v**:

VALUE	EXPRESSION
u	u
v	v

4 Click the **Spreading** tab, and in the **Equivalent thermal conductivity** list choose **Volume average**. Click **OK**.

Initial Conditions

The initial condition remain at the default value $T = 0$.

Boundary Conditions

1 Go to menu item **Physics>Boundary Settings**.

2 Select Boundaries 2 and 3, then from the **Boundary condition** list select **Thermal insulation**.

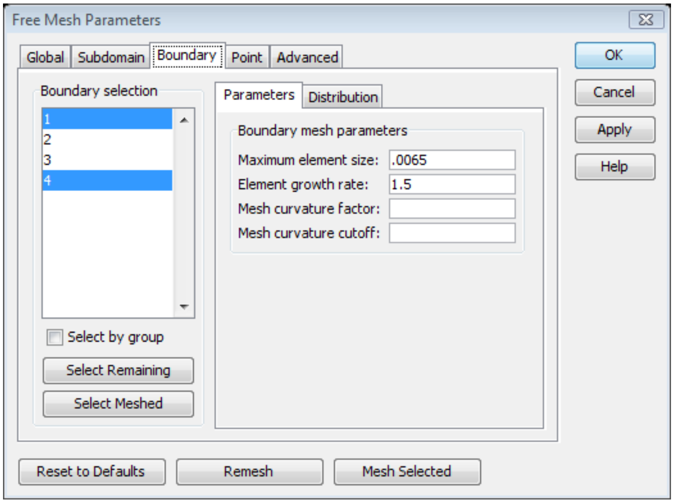
3 Select Boundary 1. From the **Boundary condition** list select **Temperature**, then in the $\mathbf{T_0}$ edit field enter `0`.

4 Select Boundary 4. From the **Boundary condition** list select **Temperature**, then in the $\mathbf{T_0}$ edit field enter `1`.

MESH GENERATION

1 Choose **Mesh>Free Mesh Parameters**.

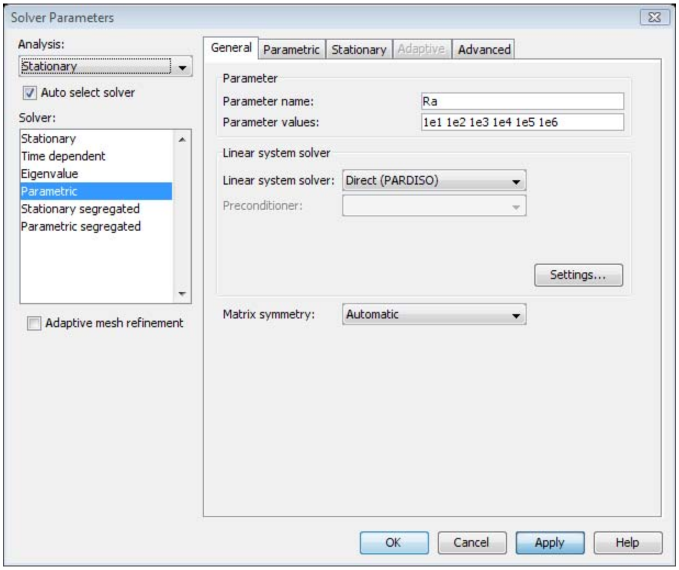
2 Click the **Boundary** tab. Select Boundaries 1 and 4. In the **Maximum element size** edit field enter `0.0065`, and in the **Element growth rate** edit field enter `1.5`. Click **Remesh**. Click **OK**.



COMPUTING THE SOLUTION

1 Select the menu item **Solve>Solver Parameters**. In the **Solver** list select **Parametric**.

2 In the **Parameter name** edit field enter `Ra`, and in the **Parameter values** edit field enter `1e1 1e2 1e3 1e4 1e5 1e6`. Click **OK**.



3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate the image in Figure 5-2 on page 287:

1 Select the menu item **Postprocessing>Plot Parameters**.

2 On the **General** page select the **Surface**, **Contour**, and **Arrow** check boxes. In the **Solution to use** list choose the appropriate value for Ra.

3 Click the **Surface** tab. In the **Predefined quantities** list select **Temperature (eshcc)**.

4 Click the **Contour** tab. In the **Predefined quantities** list select **x-velocity (chns)**. Go to the **Contour color** area, select the **Uniform color** option button, click the **Color** button, as the color choose white, and click **OK**.

5 Click the **Arrow** tab. In the **Predefined quantities** list select **velocity field (chns)**. Go to the **Arrow positioning** area. For the **Number of points**, in both the **x-points** and **y-points** edit fields enter `15`. Click **Color**, select black, then click **OK**.

6 Click **OK** to close the **Plot Parameters** dialog box.

To sequence through the different solutions as an animation, open the **Postprocessing>Plot Parameters** dialog box, click the **Animate** tab, then click the **Start Animation** button.

Free Convection in Porous Media

This example describes subsurface flow in porous media driven by density variations that result from temperature changes. The model comes from Hossain and Wilson (Ref. 1) where they use a specialized in-house code to solve this free-convection problem. This COMSOL Multiphysics example reproduces their work using the Brinkman Equations application mode and the Convection and Conduction application mode. The results of this model match those from the published study.

Model Definition

The following figure gives the model geometry. Water in a porous media slice can move within the slice but not exit from it. Temperatures vary from high to low along the outer edges. Initially the water is stagnant, but the temperature change alters density to the degree that buoyant flow ensues. The problem statement specifies that the flow is steady state.

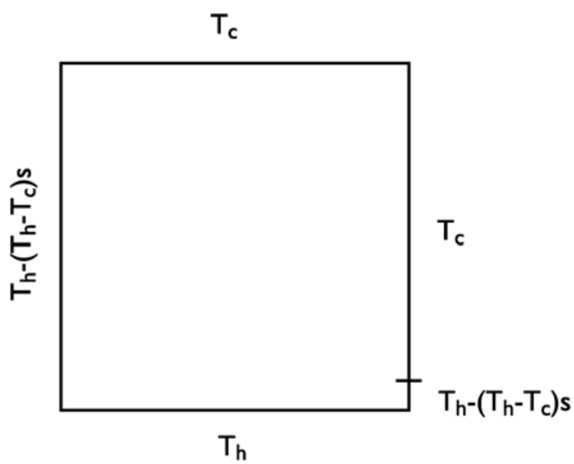


Figure 5-3: Domain geometry and boundary conditions for the heat balance in the free-convection problem. Th is a higher temperature than Tc, while s is a variable that represents the relative length of a boundary segment and goes from 0 to 1 along the segment.

You model this free-convection problem by introducing a Boussinesq buoyancy term defined with temperatures to the Brinkman equations, then link the resulting fluid velocities from the Brinkman equations to the heat transfer application mode.

The Boussinesq buoyancy term that appears on the right side of the Brinkman equation shown next accounts for the lifting force due to thermal expansion

$$-\nabla \cdot \frac{\eta}{\varepsilon}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \left(\frac{\eta}{\kappa}\mathbf{u} + \nabla p\right) = \rho_0 \mathbf{g} \beta (T - T_0) \tag{5-4}$$

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

In these expressions, T represents temperature while T_0 is a reference temperature, $\mathbf{g}$ denotes the gravity acceleration, ρ_0 gives the reference density, ε is the porosity, and β is the thermal expansion coefficient.

The heat balance comes from the conduction-convection equation

$$C_L \mathbf{u} \nabla \cdot T - \nabla \cdot (K_{\mathrm{eq}} \nabla T) = 0$$

where K_{eq} denotes the effective thermal conductivity of the fluid-solid mixture, and C_L is the fluid's volumetric heat capacity.

The boundary conditions for the Brinkman equations are all no-slip conditions. Using only velocity boundaries gives no information on the pressure within the domain, which means that the model produces estimates of the pressure change instead of the pressure field. However, without any seed information on pressure, the problem is unlikely to converge. The remedy is to arbitrarily fix the pressure at a point in the model using point settings. The boundary conditions for the Convection and Conduction application mode are the series of fixed temperatures in Figure 5-3.

Implementation: Initial Conditions for Boussinesq Approximation

The simple problem statement just given produces a strongly nonlinear problem that represents a difficult convergence task for most nonlinear solvers. Even without the new Boussinesq term, the Brinkman equations are nonlinear alone. To ease the numerical difficulties, you apply a relaxation factor damp in front of the Boussinesq term $\rho_0 \mathbf{g} \beta (T - T_0)$ in Equation 5-4 to gradually find a stable initial condition for solving the true problem. When damp = 0, the flow and temperature equations are uncoupled so the model easily converges. Then you gradually increase damp, using the previous solution as the initial guess for the next parametric step, and so on until you reach damp = 1. The iteration protocol is an easy process with COMSOL Multiphysics' parametric solver.

Results

This example reproduces a model reported by Hossain and Wilson (Ref. 1). After extracting the input data from the paper, the author constructed the model in less than an hour, including all the steps from geometry input to postprocessing of the results. Figure 5-4 shows the dimensionless temperature distribution throughout the porous media slice.

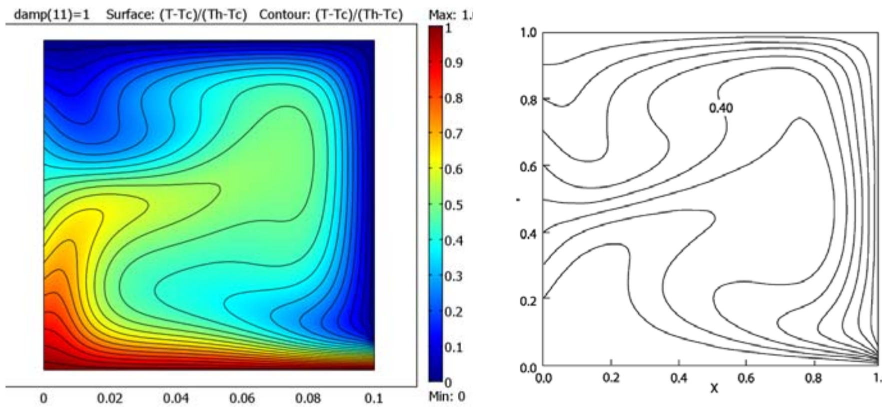


Figure 5-4: Dimensionless temperature in a porous structure subjected to temperature gradients and subsequent free convection. The COMSOL Multiphysics simulation (left) and the published results from Ref. 1 (right) are in excellent agreement.

The COMSOL Multiphysics plot (left) provides higher resolution on the results than the reproduction of the published data (right). Otherwise the two graphs are identical. Figure 5-5 gives the COMSOL Multiphysics solution for the flow field.

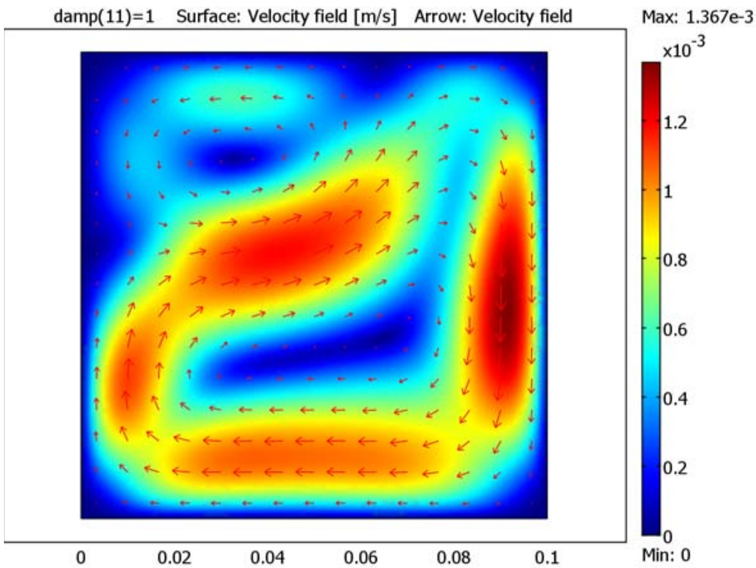


Figure 5-5: Velocity field (surface color) and velocity arrows.

Reference

1. M. Anwar Hossain and M. Wilson, “Natural convection flow in a fluid-saturated porous medium enclosed by non-isothermal walls with heat generation,” *Int. J. Therm. Sci.*, vol. 41, pp. 447–454, 2002.

Model Library path: `Earth_Science_Module/Heat_Transfer_Models/free_conv_porous`

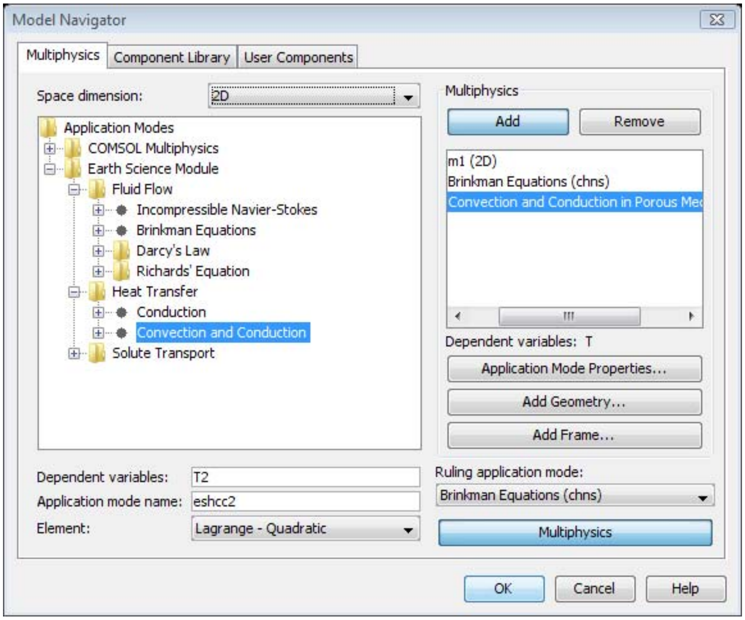
Modeling Using the Graphical User Interface

1 In the **Model Navigator**, click the **Multiphysics** button, then in the **Space dimension** list select **2D**.

2 In the list of application modes select **Earth Science Module>Fluid Flow>Brinkman Equations**. Click the **Add** button.

3 In the list of application modes select **Earth Science Module>Heat Transfer>Convection and Conduction**. Click **Add**.

4 Click **OK**.



OPTIONS AND SETTINGS

1 From the **Options** menu select **Constants**, then enter the following names, expressions, and descriptions (optional). When done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho	1e3	Density
mu	4e-4	Dynamic viscosity
cp1	4.2e3	Heat capacity
perm	1e-3	Permeability
beta	276e-6	Thermal expansion coefficient
Tc	0	Reference temperature
g	9.81	Acceleration due to gravity
damp	1	Relaxation factor

2 Select the menu item **Options>Expressions>Scalar Expressions** and add these definitions (the descriptions are optional). When done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
k1	cp1*mu/0.28	Thermal conductivity
Th	Tc+0.0527	Higher temperature

Because this is a nondimensional model, use no unit system:

1 From the **Physics** menu, choose **Model Settings**.

2 Select **None** from the **Base unit system** list in the **Model Settings** dialog box.

3 Click **OK**.

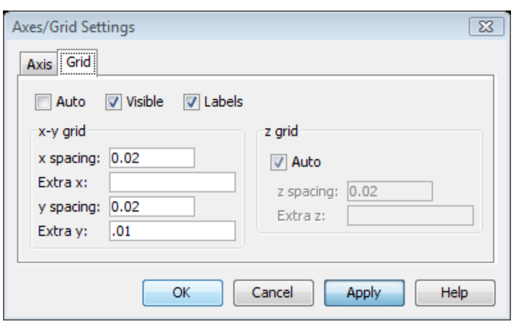
GEOMETRY MODELING

1 Select the menu item **Options>Axes/Grid Settings**. On the **Axis** page enter these settings; when done, click **OK**.

PARAMETER	VALUE
x min	-0.03
x max	0.13
y min	-0.02
y max	0.12

2 Click the **Rectangle/Square** button on the Draw toolbar, then using the cursor create a square with the corners at (0, 0) and (0.1, 0.1).

3 Return to the menu item **Options>Axes/Grid Settings**, and this time click the **Grid** tab. Clear the **Auto** check box, then in the **Extra y** edit field enter 0.01. Click **OK**.



4 Go back to the Draw toolbar and click the **Point** button. Create a point at location (0.1, 0.01).

PHYSICS SETTINGS

From the **Multiphysics** menu select **Brinkman Equations (chns)**.

Boundary Conditions

The boundary conditions default to **No slip** and need not be altered.

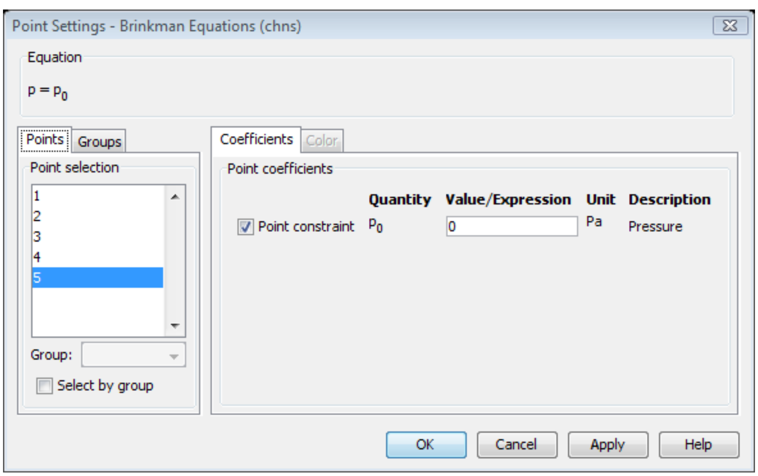
Subdomain Settings

Select the menu item **Physics>Subdomain Settings**, select subdomain 1, then enter the following specifications; when done, click **OK**.

QUANTITY	EXPRESSION
ρ	`rho`
η	`mu`
ε_p	`0.4`
κ	`perm`
Fx	`0`
Fy	`damp*rho*g*beta*(T-Tc)`

Point Settings

From the **Physics** menu choose **Point Settings**. Select point 5 and then select the **Point constraint** check box. Leave the $\mathbf{p_0}$ edit field at `0`. Click **OK**.



Initial Conditions

Leave the initial conditions will at their default values: $u = v = p = 0$.

Boundary Conditions

1 From the **Multiphysics** menu select **Convection and Conduction in Porous Media (eshcc)**.

2 Select the menu item **Physics>Boundary Settings**.

3 Select all boundaries in the list, then in the **Boundary conditions** list select **Temperature**.

4 Select Boundaries 1 and 4, then in the $\mathbf{T_0}$ edit field enter `Th-(Th-Tc)*s`; for Boundaries 3 and 5 enter `Tc` in that edit field, and for boundary 2 enter `Th`.

Subdomain Settings

1 Select the menu item **Physics>Subdomain Settings**.

2 Click the **Time/Convection** tab. Click the $\mathbf{C_L}$ **(User defined)** button. Then enter the following settings in the associated edit fields:

VALUE	EXPRESSION
C_L	`cp1*rho`
u	`u`
v	`v`

3 Click the **Spreading** tab. In the **Equivalent thermal conductivity** list select **User defined**, and in the $\mathbf{k_{eq}}$ edit field enter `k1`.

4 Click **OK**.

Initial Conditions

Keep the initial condition at the default value of $T = 0$.

MESH GENERATION

1 Select the menu item **Mesh>Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Fine**.

3 Click the **Remesh** button.

4 Click **OK**.

COMPUTING THE SOLUTION

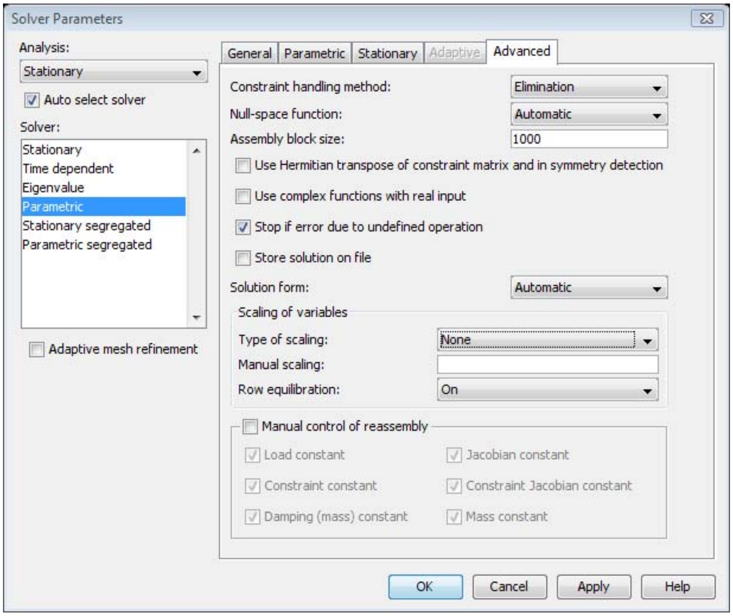
1 Select the menu item **Solve>Solver Parameters**. In the **Solver** list select **Parametric**.

2 In the **Parameter name** edit field enter `damp`, and in the **Parameter values** edit field enter `0:0.1:1`.

3 Go to **Advanced** tab and set the **Type of Scaling** to **None**.

4 Click **OK**.

5 Click the **Solve** button on the Main toolbar.



POSTPROCESSING AND VISUALIZATION

To generate Figure 5-4, follow these steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 Go to the **General** page. In the **Plot type** area select the **Surface** and **Contour** check boxes.

3 Go to the **Surface** page, and in the **Expression** edit field enter `(T-Tc)/(Th-Tc)`.

4 Go to the **Contour** page, and in the **Expression** edit field enter `(T-Tc)/(Th-Tc)`.

5 Select the **Uniform color** option button, click the **Color** button, set the color as black, then click **OK**.

6 Clear the **Color scale** check box, then click **OK**.

To generate Figure 5-5, continue with these steps:

1 While still in the **Plot Parameters** dialog box, return to the **General** page. In the **Plot type** area clear the **Contour** check box and select the **Arrow** check box. Click **Apply**.

2 Click the **Surface** tab. In the **Predefined quantities** list select **Velocity field**.

3 Click the **Arrow** tab. Verify that the **x component** edit field reads **u**, that the **y component** edit field reads **v**, and that the selected color is black. Click **OK**.

Phase Change

This example demonstrates how to model a phase change and predict its impact on a heat transfer analysis. When a material changes phase, for instance from solid to liquid, energy is added to the solid. Instead of creating a temperature rise, the energy alters the material's molecular structure. Equations for the latent heat of phase changes appear in many texts (see Ref. 1, Ref. 2, and Ref. 3) but their implementation is nonstandard. Heat consumed or released by a phase change affects fluid flow, magma movement and production, chemical reactions, mineral stability, and many other earth-science applications.

This 1D example uses the Conduction in Porous Media application mode from the Earth Science Module to examine transient temperature transfer in a rod of ice that heats up and changes to water. This example demonstrates how to handle material properties that vary as a function of temperature. A phase change with flow is the subject of the model "Freezing Soil" on page 198.

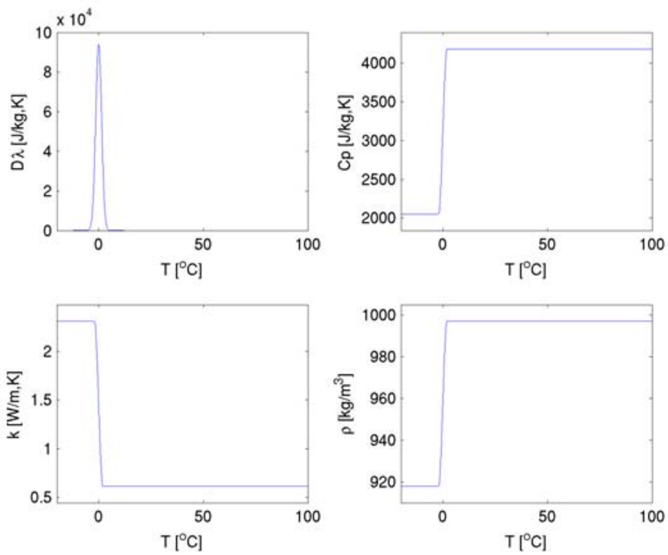


Figure 5-6: Material properties as a function of temperature.

This model proceeds as follows. First, estimate the ice-to-water phase change using the transient conduction equation with the latent heat of fusion. Next, run additional simulations to evaluate impacts of the temperature interval over which the phase change occurs. Finally, compare the solution from the analysis with the latent heat to estimates that neglect it.

Model Definition

This model describes the ice-to-water phase change along a 1-cm rod of ice. At its left end the rod is insulated, and at the other end it touches boiling water. Values for thermal properties depend on the phase. For ice, density is 918 kg/m^3, the specific heat capacity is 2052 J/(kg·K), and the thermal conductivity is 2.31 W/(m·K). For water, the density, specific heat capacity, and thermal conductivity are 997 kg/m^3, 4179 J/(kg·K), and 0.613 W/(m·K), respectively. Reference temperatures are 265 K for ice and 300 K for water. The latent heat of fusion, λ, is 333 kJ/kg. The starting temperature in the rod is –20 °C.

The conduction equation is

$$\delta_{\mathrm{ts}}\ C_{\mathrm{eq}}\frac{\partial T}{\partial t} + \nabla \cdot (-K_{\mathrm{eq}}\nabla T) \quad = \Sigma \boldsymbol{Q}\,.$$

In the equation, C_{eq} is the effective volumetric heat capacity (J/K·m^3), T is temperature (K), K_{eq} is the effective thermal conductivity (W/m·K), and $\boldsymbol{Q}$ is a heat source (W/m^3).

C_{eq} and K_{eq} typically are volume averages of the form

$$C_{\mathrm{eq}} \quad = \Sigma\theta_i\rho_i C_{pi}$$

where θ is the volumetric content, ρ equals density (kg/m^3), and C_p is the specific heat capacity (J/(K·kg)) of a liquid or a solid. In this problem, however, you modify C_{eq} to account for the latent heat of fusion so that

$$C_{\mathrm{eq}} \quad = \Sigma\theta_i\rho_i(C_{pi} + D\lambda)\,.$$

It describes latent heat using the latent heat of fusion λ (J/kg) for only the normalized pulse around a temperature transition D (K^{-1}).

The integral of D must equal unity to satisfy the following

$$\int_{-\infty}^{\infty} \rho D \lambda dT = \rho\lambda$$

such that the pulse width denotes the range between the liquidus and solidus temperatures.

The boundary conditions for this model are insulating at $x = 0$ and fixed temperature at $x = 0.01$ where

$$\begin{array}{lll} \mathbf{n} \cdot (-K_{eq} \nabla T) = 0 & \partial\Omega & \text{Origin} \\ T = T_0 & \partial\Omega & \text{Heat source} \end{array}$$

Implementation

Because the thermal properties differ between ice and water, you create a variable H, which goes from unity for water to zero for ice. In this way H amounts to the volume fraction θ of water within a model element. Therefore, the effective properties switch with the phase through multiplication with H.

The switch in H from 0 to 1 occurs over the liquid-to-solid interval using a smoothed Heaviside function. This model implements the Heaviside function with the expression `H = flc2hs(T-Ttrans,dT)`; where the transition interval for the function is dT. In this way, the pulse D is the derivative of H with respect to temperature. You can then express D with the COMSOL Multiphysics `diff` operator as in `D = diff(H,T)`.

To find out more about implementing this and other smoothing functions, see the *COMSOL Multiphysics User's Guide* under "Specifying Discontinuous Functions" on page 149 as well as the *COMSOL Multiphysics Reference Guide*.

Results

Figure 5-7 shows images of the temperature distribution predicted with latent heat for output intervals of 100 s. The system is solid ice at $t = 0$, and water content increases with time. The distributions level out around the zero temperature point because not all of the energy is going toward a temperature rise; some is being absorbed to change the molecular structure and change the phase.

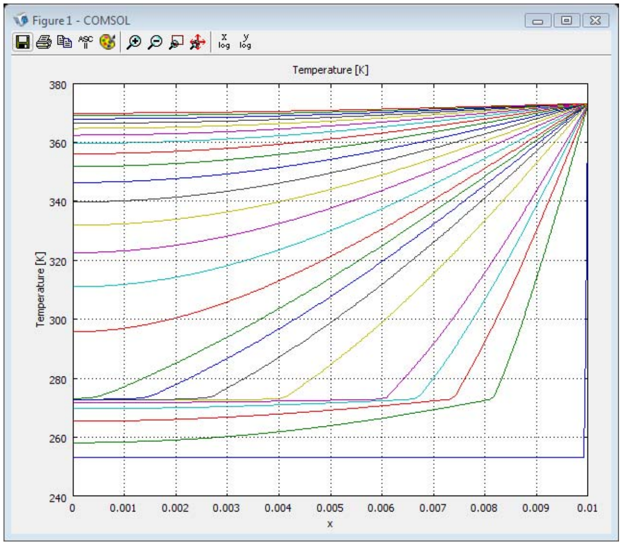


Figure 5-7: Temperature estimates with latent heat at t = 0:15:60 and120:60:1200 s.

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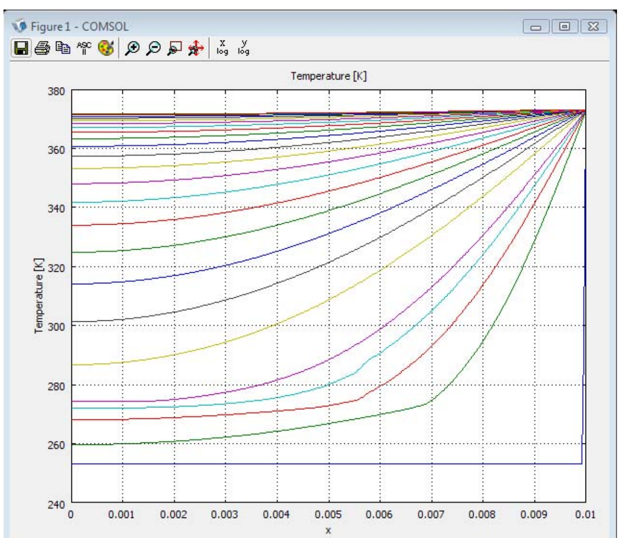


Figure 5-8: Temperature estimates without latent heat a t = 0:15:60 and120:60:1200 s.

The solution in Figure 5-8 shows temperature estimates for the simulation without latent heat. The kink in the temperature curve results from differences in the thermal properties of ice and water.

Figure 5-9 shows results for different solid-to-liquid intervals at three times. The smaller the interval, the sharper the bend in the temperature profile at zero temperature, T. In the simulations, narrowing the temperature interval to a step change, for example, comes at a large computational cost. In the figure, the results for the wide and narrow pulses compare closely.

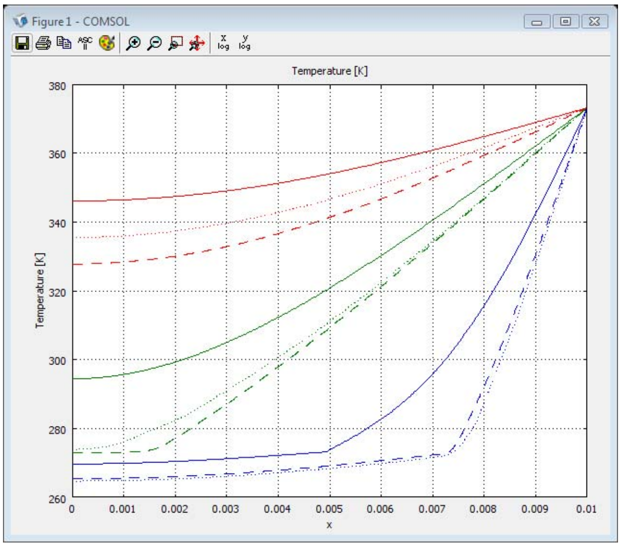


Figure 5-9: Temperature estimates for different temperature intervals for latent heat consumption. Estimates are for dT intervals of 0.1 (solid line), 0.5 (dashed line), and 2.5 (dotted line) at t = 30 s, 300 s, and 600 s.

References

1. S.E. Ingebritsen and W.E. Sanford, *Groundwater in Geologic Processes*, Cambridge University Press, 1998.

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

3. D.L. Turcotte and G. Schubert, *Geodynamics, Applications of Continuum Physics to Geological Problems*, 2nd ed., Cambridge University Press, 2002.

Model Library path: `Earth_Science_Module/Heat_Transfer/phase_change`

Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1. In the Model Navigator go to he **Space dimension** list and select **1D**.
2. In the list of application modes select **Earth Science Module>Heat Transfer>Conduction>Transient analysis**.
3. Click **OK**.

OPTIONS AND SETTINGS

1. Select the menu item **Options>Constants**, then enter the following names, expressions, and descriptions (optional); when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
T_trans	0[degC]	Transition temperature
dT	0.5[K]	Transition interval
lm	333[kJ/kg]	Latent heat of fusion

2. Select the menu item **Options>Expressions>Scalar Expressions** and define the following names and expressions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
H	flc2hs((T-T_trans)[1/K],dT[1/K])	Heaviside function
D	diff(H,T)	Temperature transition

GEOMETRY MODELING

1. Select the menu item **Draw>Specify Objects>Line**. Define the end points by going to the **x** edit field and entering `0 0.01`.
2. Click the **Zoom Extents** button on the Main toolbar to center the line in the field of view.

PHYSICS SETTINGS

Boundary conditions

1. From the **Physics** menu select **Boundary Settings**.

2 In the **Boundary selection** list select **2**, then in the **Boundary condition** list select **Temperature**.

3 To set the high temperature at the heat source go to the **Temperature** edit field and enter `100[degC]`.

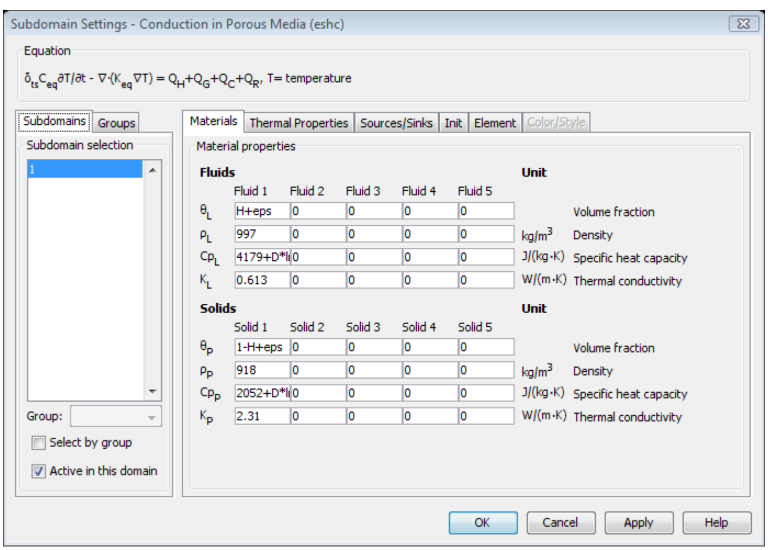
4 To accept the boundary conditions as entered, click **OK**.

Subdomain settings

1 Select the menu item **Physics>Subdomain Settings**.

2 On the **Materials** page, select Subdomain 1 and enter the following liquid (L) and solid (P) property values; when done, click **OK**.

SYMBOL	EXPRESSION
θ_L	`H+eps`
ρ_L	`997`
C_{pL}	`4179+D*lm`
K_L	`0.613`
θ_P	`1-H+eps`
ρ_P	`918`
C_{pP}	`2052+D*lm`
K_P	`2.31`



3 Click the **Init** tab and in the **T(t_0)** edit field enter `-20`.

4 Click the **Element** tab. In the **Predefined elements** list choose **Lagrange-Linear**.

The use of linear elements reduces computation time at a relatively small price in accuracy. This feature can be particularly helpful during concept-development stages, after which you might want to switch back to **Lagrange-Quadratic** elements.

MESH GENERATION

1 Click the **Initialize Mesh** button on the Main toolbar. The mesh consists of 15 elements, making it quite coarse.

2 Click the **Refine Mesh** button on the Main toolbar three times to obtain a relatively fine mesh with 120 elements.

COMPUTING THE SOLUTION

1 Select the menu item **Solve>Solver Parameters**.

2 Go to the **Times** edit field and enter `0:15:60,60:60:1200`. Click **OK**.

All the parameter values in this model have a time units of seconds, so the output time you enter here gives a total simulation time of 20 minutes.

3 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 5-7, follow these steps:

1 Select the menu item **Postprocessing>Domain Plot Parameters**.

2 Click the **Line/Extrusion** tab, then in the **Subdomain selection** list choose **1**.

3 In the **y-axis data** area go to the **Predefined quantities** list and select **Temperature**.

4 From the **Unit** list, select **°C** to display the temperature in degrees Celsius.

5 Click the **General** tab and verify that all time steps in the **Solutions to Use** list are selected.

SAVING THE FILE

To save the current model, go to the menu item **File>Save As**, enter the file name `phase_change`, then click **OK**. Also leave the model file open.

Phase Change Without Latent Heat

To analyze the impact of the latent heat terms on the phase-change model, it is useful to estimate temperatures using the same approach but without the latent heat term.

OPTIONS AND SETTINGS

From the **Options** menu select **Constants**. Find the name for latent heat (**lm**) and in the associated **Expression** edit field enter `0[kJ/kg]`. Click **OK**.

COMPUTE THE SOLUTION

Solve the model by clicking the **Solve** button in the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To create Figure 5-8, use the postprocessing sequence described for Figure 5-7 on page 306.

Phase Change for Varying Transition Intervals

Solutions to the phase-change problem vary with the range in temperatures *dT* over which you assume the phase transition occurs. To visualize the impact of different transition widths, sample results from the original simulation and compare those estimates to results from simulations with varying *dT* values.

SAMPLING THE PREVIOUS RESULTS

To creating Figure 5-9, follow these steps:

1 Reopen the model `phase_change.mph` and select the menu item **Postprocessing>Domain Plot Parameters**.
2 On the **General** page, go to the **Solutions to use** list and select output times **60**, **300**, and **600**. Select the **Keep current plot** check box.
3 Click **OK** to generate the plot; do not close the plot window.

OPTIONS AND SETTINGS

Select the menu item **Options>Constants**. Change `dT` to another value, for instance `2.5[K]`. Click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

The second part of creating Figure 5-9 is with these steps:

1 Select the menu item **Postprocessing>Domain Plot Parameters** and go to the **General** page. In the **Solutions to use** list select the same output times: **60**, **300**, and **600**.

2 Next click the **Title>Axis** button and modify the settings as appropriate. Click **OK**.

3 To complete the comparison plot, go to the **Line/Extrusion** page, click the **Line Settings** button and change the line properties to distinguish the new set of results, then click **OK**. Click **OK** to close the dialog box.

6

Multiphysics Models

Two models in 2D and 3D of the electrokinetic and magnetic fields inside a volcano highlight the multiphysics modeling capabilities in COMSOL Multiphysics and the Earth Science Module.

Electrokinetic and Magnetic Fields Inside a Volcano

This multipart example examines several coupled geophysical phenomena: the electrokinetic voltages generated as fluid moves through porous media; the magnetic field the currents produce; and the feedback from the electric field to the fluid flow. Investigating these effects is important in many applications (Ref. 1, Ref. 2, and Ref. 3) such as tracking subsurface distribution and flow of fluids, estimating reservoir properties, predicting hydrothermal flow, and establishing innovative methods for mitigating subsurface contaminants, to name a few. The models described here couple the Darcy's Law application mode of the Earth Science Module with COMSOL Multiphysics' DC Conductive Media and Magnetostatics application modes.

In the first stages of this model, fluid-flow equations are 1-way coupled to electric-field equations for a 2D geometry. Here the moving fluid generates a current that in turn generates magnetic fields, which you calculate with a COMSOL Multiphysics application mode. In the second step you compare the magnetic fields just calculated with the COMSOL Multiphysics to those predicted with Biot-Savart's law. After matching the analytic expression, you relax the restrictions of 1-way coupling and couple the fluid-flow and electric-field equations bidirectionally. The feedback from the electric field to the fluid flow equations adds electroosmotic forces to the fluid velocity.

This model is based on research carried out at the University of Leipzig and ETH Zurich. A detailed description of the underlying physics and consequences for volcanological exploration appears in Ref. 4. Finally, this example develops a 3D version of the model using an elevation model contributed by Prof. Carl Gerstenecker of the Technical University of Darmstadt (Ref. 5). Both models are available in the *Earth Science Module Model Library.*

Note: These models require the AC/DC Module.

Model Definition

Figure 6-1 shows the infiltration of rain water info a volcano conduit. The water is moving preferentially through highly permeable fractured rocks in a volcano's neck. Very little water flows in the older impermeable parts of the edifice. Measuring the distribution of voltages and magnetic fields provides insight into the internal flow regime.

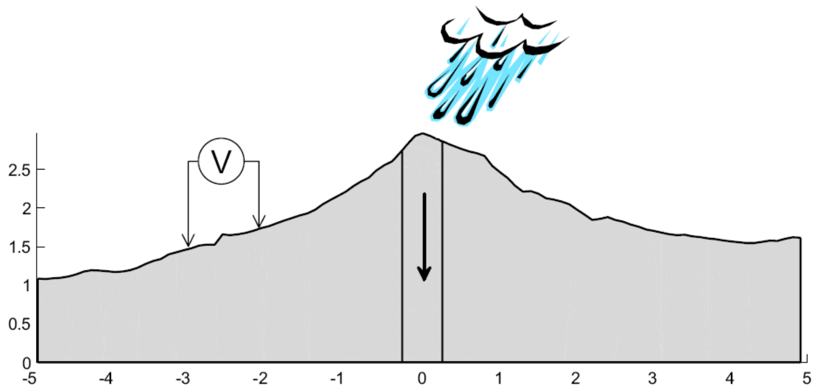


Figure 6-1: Vertical slice through a volcano with a permeable conduit.

FLUID FLOW

The fluid flow in this problem is steady so you describe it with the continuity equation

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

where $\mathbf{u}$ is a vector of directional fluid velocities.

In a first approximation, neglecting the electroosmotic drag, the fluid velocity is governed by Darcy's law

$$\mathbf{u} = -\frac{\kappa}{\eta}\nabla P$$

where κ denotes the hydraulic permeability of the porous medium, and η is the fluid's dynamic viscosity.

The boundary conditions for the hydraulic system are as follows: Infiltration occurs only at the top of the conduit assuming that water supplied to the system moves vertically under its own weight. This produces a seepage velocity of

$$u_0 = \rho g \frac{\kappa}{\eta}$$

in the y direction through the boundary. Here, ρ is the fluid density and g is gravitational acceleration. At the bottom of the conduit you assume an outflow of $-u_{\text{out}}$ (see details in section topography). All other boundaries are hydraulic insulating, $\mathbf{u} \cdot \mathbf{n} = 0$.

ELECTRIC POTENTIAL

The equation of continuity for electric potential reads

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

where $\mathbf{J}$ is current density.

Ohm's law governs the flow of electric potential. After adding the current generated by the fluid flow, the equation for current density reads

$$\mathbf{J} = -\sigma \nabla V - \alpha \nabla P = \sigma \mathbf{E} + \mathbf{J}^e$$

where σ denotes the rock's electric conductivity, and V is the electric potential.

FLOW-TO-ELECTRIC POTENTIAL COUPLING

The equation contains an electrokinetic-coupling coefficient α given by

$$\alpha = \frac{\varepsilon \zeta}{\eta F_0}$$

where ε is the dielectric permittivity, ζ denotes the zeta potential of the mineral-fluid interface, and F_0 is the formation factor, that is, the ratio between fluid and rock resistivity ($\sigma_{\text{fluid}}/\sigma$).

The electric problem is completely insulated, $\mathbf{J} \cdot \mathbf{n} = 0$. At the earth's surface, no current leaves the rock into the air. The subsurface boundaries of the modeling domain are sufficiently far away from the sources to be unaffected by changes near the surface.

POINT SETTINGS FOR A UNIQUE SOLUTION

Because both the hydraulic and the electric problems use only Neumann boundary conditions, you make the problem unique by setting $p = 0$, $V = 0$ at an arbitrary point.

MAGNETIC-FIELD EQUATIONS

To calculate the magnetic field or magnetic flux density that corresponds to the electric current field resulting from the hydraulic flow, use the quasi-static approximation

$$\nabla \times \mathbf{E} = 0 .$$

Further, using Ampere's law with the multiphysics definition for current density gives

$$\nabla \times \mathbf{H} = \mathbf{J} = \sigma\mathbf{E} + \mathbf{J}^e .$$

The governing equation for the magnetic field therefore reads

$$\nabla \times (\sigma^{-1}(\nabla \times \mathbf{H} - \mathbf{J}^e)) = 0 .$$

Here the only boundary condition needed is the electric insulation.

In the postprocessing steps described later in this chapter you compare these magnetic-flux estimates to those obtained with Biot-Savart's law.

2D Model with Topography and Electroosmotic Force

A realistic geological model would need to account for two additional features: the effect of topography and the feedback of the electric field on the hydraulic flow.

In reality, the electric field influences the flow field and exerts electroosmotic drag. Moreover, topographical nuances figure prominently in generating the electric field. With a sloping surface you can no longer assume that all rainfall penetrates the ground surface. Instead some rainfall runs off, which affects the flow field.

ELECTROOSMOTIC DRAG

To account for electroosmotic drag in Darcy's law, use the reciprocity relations of Onsager (Ref. 2):

$$\mathbf{u}_{\text{new}} = -\frac{\kappa}{\eta}\nabla P - \alpha\nabla V .$$

Here you implement the electric-field component by including it as a source term in COMSOL Multiphysics' Darcy's Law application mode. You also define a modified velocity vector using subdomain expressions, which you plot during postprocessing.

TOPOGRAPHY

Users often prefer to obtain realistic topography models by importing geometries. Topography models can be conveniently imported by using one of COMSOL

Multiphysics' CAD interfaces (for example DXF in 2D or, using the CAD Import Module, most of the popular 3D CAD formats, including IGES, STEP, SAT, and Parasolid files). In addition, COMSOL Script provides unlimited flexibility to read in data in ASCII or binary format. In this case you import the volcano geometry as a DXF file in the COMSOL Multiphysics user interface.

The geometry features three major fracture zones: one main conduit and two parasitic conduits. One of the parasitic conduits developed itself fully to the surface, while the other one stalled and produced a cryptodome. Because the fractures zones are highly permeable, rainfall penetrates preferentially through the conduits that intersect the surface and exits the system through the conduits at depth. Owing to the topography, only part of a rainfall penetrates the ground surface and a fraction runs off. Assuming the infiltration into the ground is a function of topographic slope, the fluid velocity crossing the boundary is the rainfall rate, u_0, multiplied by the vertical component of the normal vector to the boundary, n_y.

At steady state, the flow moving out of the system at any point (the outflow) must equal the total rainfall entering at the ground surface (influx) divided by the outflow boundary length (outlength). In this example, you automate the calculation using integration coupling variables.

$$u_{\text{in}} = u_0 n_y \qquad \text{outflow} = \frac{\text{influx}}{\text{outlength}} = \frac{\int_{\text{in}} u_0 n_y ds}{\int_{\text{out}} ds}$$

Results—2D Model with Topography and Electroosmotic Force

Figure 6-2 illustrates the COMSOL Multiphysics solution for fluid pressure and fluid velocities in the volcano where a 2-way coupling exists between fluid flow and electric potential. The fluid moves primarily within the fractured conduits reaching the surface.

The model modifies the fluid velocities to include a term that accounts for electroosmotic drag generated by the electric field.

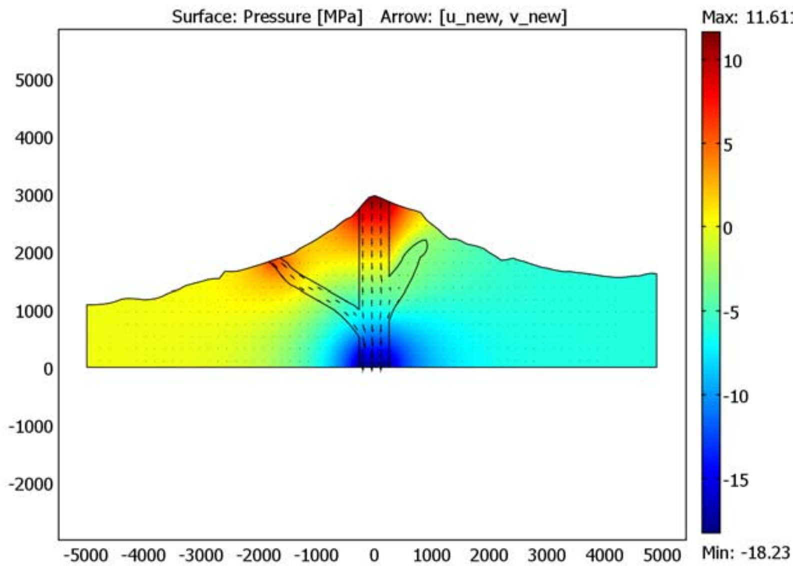


Figure 6-2: Solution for pressure distribution (surface plot) and velocities (arrows).

Figure 6-3 shows the electric self potential and the total electric current. Moving fluids initiate the electric potential. The plot marks negative anomalies at the top of the two outcropping domes. Positive potential is created at the bottom of the model, and at the top the cryptodome acts as a collector of hydraulic and electric flux.

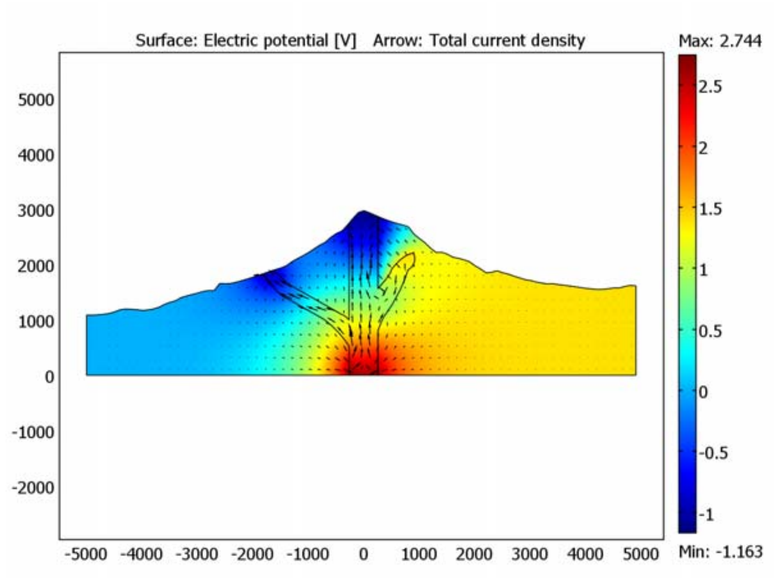


Figure 6-3: Solution for electric potential (surface plot) and current density (arrows).

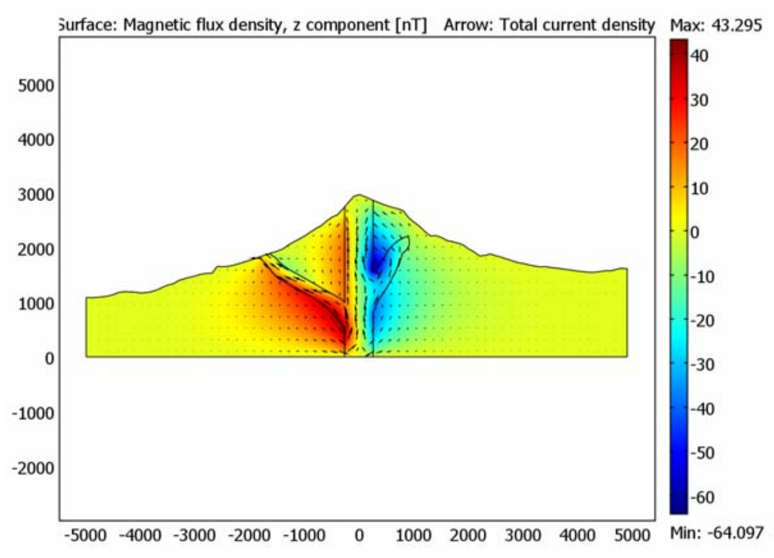


Figure 6-4: Solution for magnetic flux (surface plot) and current density (arrows).

Figure 6-4 plots the magnetic flux density with the current density. The flux densities are highest along the boundaries of the permeable conduits. The field is directed out of the plane on the left edges and into the plane on the right edge.

Magnetic Field Postprocessing—Biot-Savart's Law

In this section you calculate the magnetic field with the Biot-Savart formula and compare these estimates to the COMSOL Multiphysics solution just reported. The comparison provides a good check for consistency and accuracy.

Assuming constant magnetic permeability $\mu_r = 1$, you can calculate the magnetic flux density for an arbitrary current system $\mathbf{j}$ with Biot-Savart's law

$$\mathbf{B}(\mathbf{r}_0) = \frac{\mu_0}{4\pi}\int\frac{\mathbf{j}\times(\mathbf{r}_0-\mathbf{r})}{|\mathbf{r}_0-\mathbf{r}|}d\mathbf{r}$$

where $\mu_0 = 4\pi\cdot 10^{-7}$ V·s/(A·m) is the permeability of free space. For a point $r_0 = (x_0, y_0)$ in the xy-plane, you obtain the field components

$$B_x = \frac{\mu_0}{4\pi}\int\frac{-j_x z}{((x_0-x)^2+(y_0-y)^2+z^2)^{3/2}}dxdydz$$

$$B_y = \frac{\mu_0}{4\pi}\int\frac{j_y z}{((x_0-x)^2+(y_0-y)^2+z^2)^{3/2}}dxdydz$$

$$B_z = \frac{\mu_0}{4\pi}\int\frac{j_x(y_0-y)-j_y(x_0-x)}{((x_0-x)^2+(y_0-y)^2+z^2)^{3/2}}dxdydz$$

B_x and B_y become zero when integrating in the z direction. For the remaining component, the identity

$$\int_{-\infty}^{\infty}\frac{1}{\sqrt{a^2+z^2}^3}dz = \frac{2}{a^2}$$

applies. Combining the expressions gives

$$B_z(x_0, y_0) = \frac{\mu_0}{2\pi}\int\frac{j_x(y_0-y)-j_y(x_0-x)}{(x_0-x)^2+(y_0-y)^2}dxdy\ . \tag{6-1}$$

To calculate the expression in Equation 6-1 for an arbitrary point (x_0, y_0) you use the COMSOL Multiphysics interpolation command `postint`. You create the string to be integrated with the `sprintf` command. To create Figure 6-5 with COMSOL Script or MATLAB, see the section “Modeling Using the Programming Language” on page 329.

Results—Postprocessing the Magnetic Field

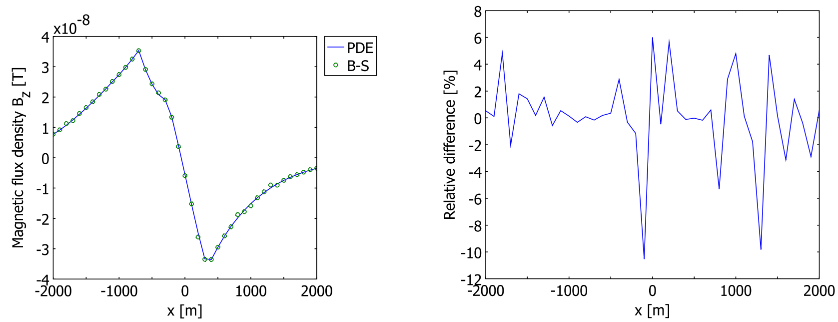


Figure 6-5: Left plot—Comparison of the B_z field evaluated directly from the PDE (solid line) and the Biot-Savart integration (o). Right plot—Relative difference between PDE solution and the integrated result. The rms error for the 17,700-element mesh is 4%.

Figure 6-5 plots the COMSOL Multiphysics solution and the Biot-Savart estimates. The results agree well with an average percent difference of 4% along the profile. In the example with 17,700 elements the calculation of Biot-Savart requires about twice as much time as solving the magnetic PDE directly.

3D Model of Fluid Flow, Electrostatics, and Magnetostatics

In a 3D model of coupled fluid flow, electrostatics, and magnetostatics for an approximately cylindrical/axisymmetric geometry, toroidal fields form around the volcanic conduits where fluid flow is fast. To examine these effects, extend the 2D model to 3D. You can review the model file and postprocess the results by opening the file `volcano3d.mph` in the *Earth Science Module Model Library*. The author created the 3D geometry using data provided by Carl Gerstenecker of TU Darmstadt based on his work with Tiede, Läufer, Wrobel, and Steineck (Ref. 5).

Results—3D Model of Fluid Flow, Electrostatics, and Magnetostatics

Figure 6-6 is a cutaway view of the COMSOL Multiphysics solution for 3D fluid pressure and fluid velocities in the volcano where fluid flow and electric potential are 2-way coupled. Again the fluid moves primarily within the fractured conduits to reach the surface. The fluid velocities are driven by gradients in pressure and electric potential. The magnetic field results from the electric current density. The visible toroidal effects center on the fast flow around the conduit.

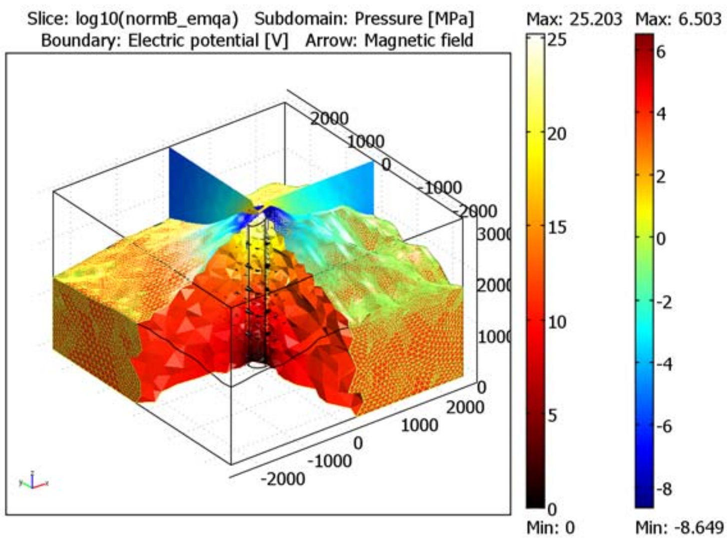


Figure 6-6: COMSOL Multiphysics solution for coupled fluid flow, electrostatics, and magnetostatics in a volcano.

References

1. P.M. Adler, PJ.L Le Mouël, and J. Zlotnicki, "Electrokinetic and magnetic fields generated by flow through a fractured zone: a sensitivity study for La Fournaise volcano," *Geophys. Res. Lett.*, pp. 26:795–798, 1999.

2. L. Onsager, "Reciprocal relations in irreversible processes," *Phys. Rev.*, vol. 37, pp. 405–426, 1931.

3. J. Zlotnicki and Y. Nishida, "Review on morphological insights of selfpotential anomalies on volcanoes," *Reviews in Geophysics*, vol. 24, pp. 291–338, 2003.

4. S. Friedel, “Numerical simulation of electrokinetic and magnetic fields resulting from water flow in volcanic systems,” *J. Geophys. Res.*, submitted for publication.

5. C. Gerstenecker, C. Tiede, G. Läufer, B. Wrobel, and D. Steineck, *Proc. 1st Ass. EGU*, 2004.

Model Library path: `Earth_Science_Module/Multiphysics/volcano_2d`

Modeling Using the Graphical User Interface—2D Model

MODEL NAVIGATOR

1 Open the **Model Navigator**, and in the **Space dimension** list select **2D**.

2 In the list of application modes select **Earth Science Module>Fluid Flow>Darcy’s Law>Pressure analysis**.

3 Click the **Multiphysics** button.

4 Click the **Add** button to include the Darcy’s application mode in the model.

5 In the list of application modes select **COMSOL Multiphysics>Electromagnetics>Conductive Media DC**, then click **Add**.

6 In the list of application modes select **AC/DC Module>Statics>Magnetostatics>In-Plane Induction Currents, Magnetic Field**, then click **Add**.

7 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu select **Constants**, the enter the following names and expressions; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
sigma1	0.1[S/m]	Electric conductivity, permeable fracture
alpha1	5.0e-9[(F/m)*V/(Pa*s)]	Electrokinetic-coupling coefficient, permeable fracture
kappa1	1.0E-10[m^2]	Hydraulic permeability, permeable fracture
sigma2	0.01[S/m]	Electric conductivity, impermeable parts

NAME	EXPRESSION	DESCRIPTION
alpha2	5.0e-9[F*V/(Pa*s*m)]	Electrokinetic-coupling coefficient, impermeable parts
kappa2	1.0e-12[m^2]	Hydraulic permeability, impermeable parts
eta	8.9e-3[Pa*s]	Dynamic viscosity
rho	1000[kg/m^3]	Density
g	9.82[m/s^2]	Acceleration due to gravity
u0	rho*g*kappa1/eta	Seepage velocity

2 From the **Options** menu select **Expressions>Subdomain Expressions**.

3 Enter the following names and expressions to define new directional components of fluid velocity and a resulting total velocity that account for electroosmotic drag:

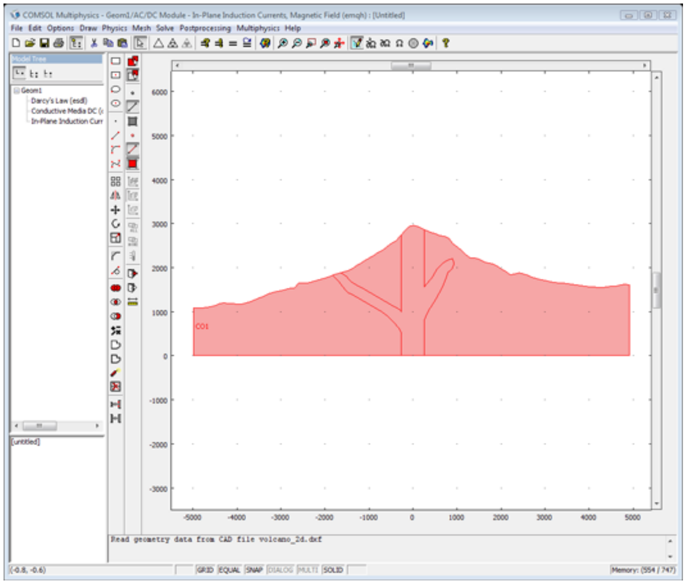
NAME	EXPRESSION FOR SUBDOMAINS 1, 3, 4	EXPRESSION FOR SUBDOMAIN 2
u_new	u_esdl-alpha1*Vx	u_esdl-alpha2*Vx
v_new	v_esdl-alpha1*Vy	v_esdl-alpha2*Vy
U_new	sqrt(u_new^2+v_new^2)	sqrt(u_new^2+v_new^2)

GEOMETRY MODELING

1 Import the volcano geometry from a DXF file. Select the menu item **File>Import>DXF File**. Find the folder `COMSOL/Earth_Science_Module/Multiphysics` and then select the file `volcano.dxf`.

2 Accept the default settings for the geometry import. Click **OK**.

3 Click the **Coerce to Solid** button on the Draw toolbar.



PHYSICS SETTINGS—DARCY'S LAW

From the **Multiphysics** menu select **Darcy's Law (esdl)**.

Application Mode Properties

1 From the **Physics** menu select **Scalar Variables**.

2 In the **Description** column look for **Elevation/vertical axis**, and in the corresponding **Expression** edit field change the entry to `0`. Click **OK**.

Subdomain Settings

1 From the **Physics** menu select **Subdomain Settings**.

2 Enter the settings from the following table; when done, click **OK**.

SETTINGS	SUBDOMAINS 1, 3, 4	SUBDOMAIN 2
κ_s	`kappa2`	`kappa1`
η	`eta`	`eta`
Q_s	`alpha2*(Vxx+Vyy)`	`alpha1*(Vxx+Vyy)`

Boundary Conditions

For the boundary condition you need two integration-coupling variables.

1 From the **Options** menu, select **Integration Coupling Variables>Boundary Variables**. Enter the following coupling variables, each on its own row in the table; when done, click **OK**.

BOUNDARIES	NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
35–37, 56–61	`influx`	`u0*ny`	4	yes
54	`outlength`	1	4	yes

2 From the **Physics** menu, select **Boundary Settings**.

3 Enter the following settings for the specified boundaries; when done, click **OK**.

SETTINGS	BOUNDARIES 35–37, 56–61	BOUNDARY 54	ALL OTHERS
Boundary condition	Inward flux	Inward flux	Zero flux/Symmetry
N_0	`u0*ny`	`ny*influx/ outlength`	

Because influx and outlength are integration coupling variables, COMSOL Multiphysics considers the unit for the inward flux across Boundary 54 to be inconsistent with the model's base unit system. You can disregard this warning.

Point Settings

1 From the **Physics** menu select **Point Settings**.

2 Select Point 2 and in the **Pressure(s)** edit field enter `0`. Click **OK**.

PHYSICS SETTINGS—CONDUCTIVE MEDIA DC

From the **Multiphysics** menu select **Conductive Media DC (dc)**.

Subdomain Settings

1 From the **Physics** menu select **Subdomain Settings**.

2 Enter the following settings; when done, click **OK**.

SETTINGS	SUBDOMAIN 1, 3, 4	SUBDOMAIN 2
σ (isotropic)	`sigma2`	`sigma1`
$\mathbf{J}$	`[-px*alpha2, -py*alpha2]`	`[-px*alpha1, -py*alpha1]`

Boundary Conditions

1 From the **Physics** menu select **Boundary Settings**.

2 Select all the boundaries, and in the **Boundary condition** list select **Electric insulation**.

3 Click **OK**.

Point Settings

To make the system well defined, you must give the potential some reference value at a given point. In this case you lock the potential at Point 2.

1 From the **Physics** menu, select **Point Settings**.
2 In the **Point selection** list select **2**.
3 Click the **Electric potential** button, and make sure the electric potential is set to 0.
4 Click **OK**.

PHYSICS SETTINGS—IN-PLANE CURRENTS, MAGNETIC FIELD

From the **Multiphysics** menu select **In-Plane Currents, Magnetic Field (emqh)**.

Subdomain Settings

1 From the **Physics** menu, select **Subdomain Settings**.
2 Enter the following settings; when done, click **OK**.

SETTINGS	SUBDOMAINS 1, 3, 4	SUBDOMAIN 2
σ (isotropic)	`sigma2`	`sigma1`
$\mathbf{J}$	`[-px*alpha2, -py*alpha2]`	`[-px*alpha1, -py*alpha1]`

Boundary Conditions

1 From the **Physics** menu, choose **Boundary Settings**.
2 Select all boundaries, and in the **Boundary condition** list select **Electric insulation**.
3 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.
2 Click the **Boundary** tab.
3 Select all interior boundaries (the boundaries on the volcano surface) and the outlet boundary (all boundaries except for 1, 2, 63, and 112).
4 In the **Maximum element size** edit field, type `20`.
5 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

Click the **Solve** button on the Main toolbar.

Modeling Using the Programming Language

To create Figure 6-5, use the following code with COMSOL Script or MATLAB. The script is also available as the M-file `volcano_2d_Bz_plots.m` located in the same directory as the model MPH-file (see the Model Library path on page 324).

```
% Create a set of coordinates along a line in the x direction
% at an altitude of 1000 m
x0 = -2000:100:2000;
y0 = x0*0+1000;

% Evaluate the Biot-Savart integral for each point
for i = 1:length(x0)
  st = sprintf(['2e-7*(Jx_dc*(%f-y)-Jy_dc*(%f-x))/' ...
  '((%f-x)^2+(%f-y)^2)'],y0(i),x0(i),x0(i),y0(i));
  Bz(i) = postint(fem,st);
end

% For comparison, evaluate the magnetic field directly from
% the COMSOL Multiphysics solution
Bz2 = postinterp(fem,'Bz_emqh',[x0;y0]);

figure, plot(x0,Bz2,x0,Bz,'o');
xlabel('x [m]');
ylabel('Magnetic flux density B<sub>z</sub> [T]');
legend('PDE','B-S');

diff = 100*(Bz-Bz2)./Bz2;
figure, plot(x0,diff);
xlabel('x [m]');
ylabel('Relative difference [%]');
```

Model Library path: `Earth_Science_Module/Multiphysics/volcano_3d`

Modeling Using the Graphical User Interface—3D Model

MODEL NAVIGATOR

1 In the **Model Navigator**, open the **Earth Science Module** folder and select **Fluid Flow>Darcy's Law>Pressure analysis**.

2 Click **Add**.

3 In the **AC/DC Module** folder, open the **Statics** folder. Select and add, in turn, **Conductive Media DC** and **Magnetostatics** application modes.

4 Click **OK**.

GEOMETRY MODELING

1 From the **File** menu, choose **Import>CAD Data From File**.

2 In the **Import CAD Data From File** dialog box, make sure that the **COMSOL Multiphysics file** or **All 3D CAD files** is selected in the **Files of type** list.

3 From the `models/Earth_Science_Module/Multiphysics` directory under the COMSOL Multiphysics installation folder, locate the `vulcano_3d.mphbin` file and click **Import**.

OPTIONS AND SETTINGS

1 From the **Options** menu, choose **Constants**.

2 Make the following entries in the **Constants** dialog box; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
sigma1	0.01[S/m]	Electric conductivity, permeable fracture
alpha1	1e-8[(F/m)*V/(Pa*s)]	Electrokinetic-coupling coefficient, permeable fracture
kappa1	1e-12[m^2]	Hydraulic permeability, permeable fracture
sigma2	0.1[S/m]	Electric conductivity, impermeable parts
alpha2	1e-8[(F/m)*V/(Pa*s)]	Electrokinetic-coupling coefficient, impermeable parts
kappa2	1e-10[m^2]	Hydraulic permeability, impermeable parts
eta	8.9e-3[Pa*s]	Dynamic viscosity
rho	1000[kg/m^3]	Density
g	9.82[m/s^2]	Acceleration due to gravity
u0	rho*g*kappa2/eta	Seepage velocity

PHYSICS SETTINGS

Subdomain Settings—Darcy's Law

1 From the **Multiphysics** menu, select **Darcy's Law (esdl)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 2, then clear the **Active in this domain** check box.

4 Select Subdomain 1, then type `kappa1` in the **Saturated permeability** edit field.

5 Select Subdomain 3, then type `kappa2` in the **Saturated permeability** edit field.

6 Select both Subdomain 1 and Subdomain 3.

7 Enter `rho` for the **Density** and `eta` for the **Viscosity**.

8 Click **OK**.

Boundary Conditions—Darcy's Law

1 From the **Physics** menu, select **Boundary Settings**.

2 Select the bottom surface of the cylinder in the geometry or select Boundary 12 from the **Boundary selection** list.

3 From the **Boundary conditio**n list, select **Pressure**. Leave the specified pressure at its default zero value.

4 Select the cylinder's upper surfaces in the geometry or select Boundary 13 from the **Boundary selection** list.

5 From the **Boundary condition** list, select **Inward flux**. Set the **Inward flux** to `-nz*u0`.

6 Click **OK**.

Subdomain Settings—Conductive Media DC

1 From the **Multiphysics** menu, select **Conductive Media DC (emdc)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 2, then clear the **Active in this domain** check box.

4 Select Subdomain 1. Enter `sigma1` in the **Electric conductivity** edit field.

5 In the edit fields for the **External current density**, enter `-alpha1*px`, `-alpha1*py`, and `-alpha1*pz`.

6 Select Subdomain 3. Enter `sigma2` in the **Electric conductivity** edit field.

7 In the edit fields for the **External current density**, enter `-alpha2*px`, `-alpha2*py`, and `-alpha2*pz`.

8 Click **OK**.

Boundary Conditions—Conductive Media DC

1 From the **Physics** menu, select **Boundary Settings**.

2 In the **Boundary Conditions** dialog box, select all boundaries and set the boundary condition to **Electric insulation**.

3 Click **OK**.

Point Settings—Conductive Media DC

1 From the **Physics** menu, select **Point Settings**.

2 Select Boundary 5 and click the $\mathbf{V_0}$ option button. Leave the potential at `0`.

3 Click **OK**.

Subdomain Settings—Magnetostatics

1 From the **Multiphysics** menu, select **Magnetostatics (qa)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomains 1and 3.

4 In the edit fields for the **External current density**, enter `Jx_emdc`, `Jy_emdc`, and `Jz_emdc`.

5 Leave the default settings for Subdomain 2.

6 Click **OK**.

Boundary Conditions—Magnetostatics

Use the default boundary settings for the Magnetostatics application mode.

Application Mode Properties—Magnetostatics

You need to turn on the gauge fixing manually for this model, because it uses other solver settings than the default settings for the 3D Magnetostatics application mode, which provide numerical gauge fixing through the SOR gauge and SORU gauge pre- and postsmoothers.

1 From the **Physics** menu, choose **Properties**.

2 In the **Application Mode Properties** dialog box, select **On** from the **Gauge fixing** list.

3 Click **OK**.

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 On the **Global** page, select **Coarse** from the **Predefined mesh sizes** list.

3 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION

Because the application modes are coupled only in one direction, you can solve them in sequence to reduce the memory consumption.

1 From the **Solve** menu, select **Solver Parameters**.

2 From the list of **Linear system solver**, select **GMRES**.

3 Set the **Drop tolerance** to `0.05`.

4 Click **OK** to close the **Solver Parameters** dialog box.

5 From the **Solve** menu, select **Solver Manager**.

6 On the **Solve For** page, select only the **Darcy's Law (esdl)** application mode.

7 Click **Apply**.

8 Click the **Script** tab. Click the **Add Current Solver Settings** button.

9 Type `fem1=fem0;` in the script window to store the current solution.

10 Click the **Initial Value** tab.

11 In the **Initial value** area, click the **Initial value expression evaluated using stored solution** button.

12 In the **Values of variables not solved for and linearization point** area, click the **Stored solution** button.

13 Click the **Solve For** tab. Select only the **Conductive Media DC (emdc)** application mode.

14 Click **Apply**.

15 Click the **Script** tab. Click the **Add Current Solver Settings** button.

16 Type `fem1=fem0;` in the script window to store the current solution.

17 Click the **Solve For** tab. Select only the **Magnetostatics (emqa)** application mode.

18 Click **Apply**.

19 Click the **Script** tab. Click the **Add Current Solver Settings** button.

20 Select the **Solve using a script** check box, then click **OK**.

21 Click the **Solve** button ono the Main toolbar to start the simulation.

POSTPROCESSING AND VISUALIZATION

The default visualization shows a pressure slice plot. To reproduce the plot shown in Figure 6-6, following these steps:

1 From the **Postprocessing** menu, select **Plot Parameters**.

2 Click the **Subdomain** tab. Select the **Subdomain plot** check box.

3 From the **Predefined quantities** list, select **Darcy's Law (esdl)>Pressure**. From the **Unit** list, select **MPa**.

4 From the **Colormap** list, select **hot**.

5 Click the **Boundary** tab. Select the **Boundary plot** check box

6 From the **Predefined quantities** list, select **Conductive Media DC (emdc)>Electric potential**.

7 In the **Coloring and fill** frame, select **Wireframe** from the **Fill style** list.

8 Click the **Arrow** tab. Select the **Arrow plot** check box.

9 From the **Predefined quantities** list on the **Subdomain Data** page, select **Magnetostatics (emqa)>Magnetic field**.

10 In the **Arrow positioning** frame, set the **Number of points** in x, y, and z to `21`, `21`, and `7`, respectively

11 In the **Arrow parameters** frame, click the **Color** button. In the **Arrow Color** dialog box, select black, then click **OK**.

12 Click the **Slice** tab. Select the **Slice plot** check box.

13 In the **Expression** edit field, type `log10(normB_emqa)`.

14 In the **Slice positioning** frame, set the **Number of levels** for x, y, and z to `1`, `0`, and `0`, respectively.

15 In the **Slice color** frame, clear the **Color scale** check box.

16 Click the **General** tab.

17 To look into the volcano, exclude part of the geometry in the postprocessing. Select the **Element selection** check box and enter `x>0|y>0` in the **Logical expression for inclusion** edit field. This only includes parts with positive x- or y-coordinates, cutting away one quarter of the geometry.

18 Click **OK** to create the plot.

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