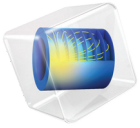

INTRODUCTION TO

Subsurface Flow Module

5.5

COMSOL

Introduction to the Subsurface Flow Module

Version: COMSOL 5.5

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Contents

Introduction

The Subsurface Flow Module extends the COMSOL Multiphysics modeling environment to the quantitative investigation of geophysical and environmental phenomena. It is designed for researchers, engineers, developers, teachers, and students, and it suits both single-physics and multiphysics modeling. The earth makes up a giant laboratory filled with an unlimited array of basic physics and multiphysics interactions. Whether in concert or alone, these physical phenomena alter our access to important resources, affect the quality of the environment, and shape the ground beneath our feet.

The contents of the Subsurface Flow Module are a set of fundamental building blocks which cover a wide array of physics questions. The physics interfaces it offers work on their own or linked to each other. They can also be coupled to physics interfaces already built into COMSOL Multiphysics, or to new equations you create. Because COMSOL Multiphysics removes the complications of writing your own code, it is our hope that you will use the Subsurface Flow Module as a springboard to investigate a rich variety of physics modeling.

The Subsurface Flow Module includes physics interfaces geared to earth-science investigations as well as a library of examples that address a range of problems. The available ready-to-run applications demonstrate a range of the included features, and also provide insight into COMSOL Multiphysics modeling in general. Each application comes with step-by-step instructions to reproduce it in the graphical user interface along with any data or additional files needed to build it on your own. Those who are unfamiliar with some of the equations or computational techniques included in the module should find the applications and the documentation extremely beneficial.

The physics interfaces, options, and functionalities in this module are tailored to account for geologic processes. The Heat Transfer interfaces, for example, include options to automate the calculation of effective thermal properties for multicomponent systems. The fluid flow equations represent a wide range of possibilities. Included are Richards' equation, which describes nonlinear flow in variably saturated porous media. The options for saturated porous media include Darcy's law for slow flow and the Brinkman equations where shear is nonnegligible. The Laminar Flow and Creeping Flow interfaces cover free flows at different Reynolds numbers. The module also treats the transport of chemical species and their reactions. The Transport of Diluted Species interface account for the transport of species in solid, liquid, and gas phases in free flow, saturated, and partially saturated porous media. A number of the examples in the application library link these physics interfaces together.

Subsurface Flow Module Physics Interfaces

The Subsurface Flow Module contains a number of physics interfaces that predefine equations or sets of equations adapted to earth-science applications. You can take the equations in these physics interfaces and their variables and then modify them, link them together, and couple them to physics interfaces represented elsewhere in COMSOL Multiphysics.

Figure 1 shows the group of physics interfaces available with this module in addition to the COMSOL Multiphysics basic license. Use these interfaces to model chemical species transport, fluid flow, heat transfer and solid mechanics, to make modeling easier, something that is briefly discussed next. See also Physics Interface Guide by Space Dimension and Study Type.

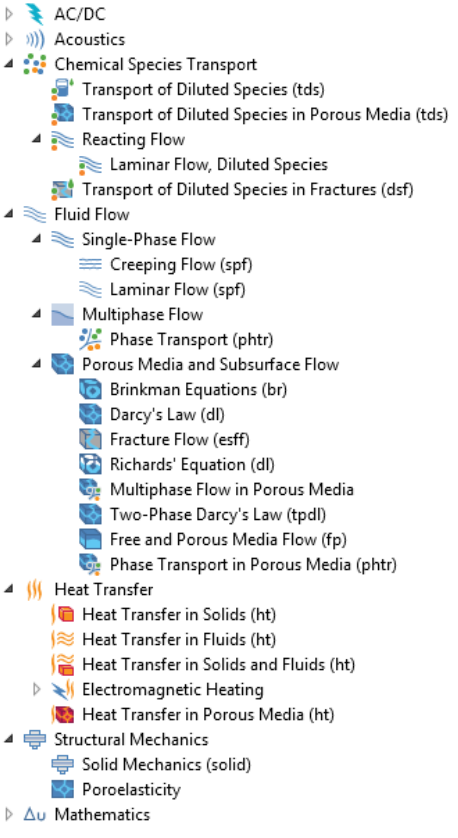

Figure 1: The physics interfaces for the Subsurface Flow Module as shown in the Model Wizard for a 3D application.

The module handles time-dependent and stationary problems for 1D, 2D, and 3D geometries with axisymmetry for 1D and 2D. The predefined physics interfaces cover four main categories: Chemical Species Transport ( ), Fluid Flow ( ), Heat Transfer ( ), and Structural Mechanics ( ), as discussed in the next pages.

Chemical Reaction and Mass Transport

The Transport of Diluted Species interface ( ) simulates chemical species transport through convection (when coupled to fluid flow), diffusion, and reactions, for mixtures where one component, a solvent, is present in excess.

The Transport of Diluted Species in Porous Media interface ( ) is tailored to model solute transport in saturated and partially saturated porous media. This physics interface characterizes the rate and transport of individual or multiple and interacting chemical species for systems containing fluids, solids, and gases. The equations supply predefined options to describe mass transfer by convection, adsorption, dispersion, diffusion, volatilization and reactions. You define the convective velocity from either of the included physics interfaces, or you set it to a predefined velocity profile.

The Laminar Flow, Diluted Species interface ( ) under the Reacting Flow branch combines the functionality of the Single-Phase Flow and Transport of Diluted Species interfaces. This multiphysics interface is primarily applied to model flow at low to intermediate Reynolds numbers in situations where the mass transport and flow fields are coupled.

The Transport of Diluted Species in Fractures interface ( ) is used to model the transport of a solutes along thin porous fractures, taking into account diffusion, dispersion, convection, and chemical reactions. The fractures are defined by boundaries in 2D and 3D, and the solutes are diluted in a solvent. The mass transport equation solved along the fractures is the tangential differential form of the convection-diffusion-reaction equation. Different effective diffusivity models are available.

Fluid Flow

Subsurface flows usually occur at low Reynolds numbers. The Reynolds number (Re) is a measure of the ratio of the fluid viscous to the inertial forces acting on the fluid and is given by: $\mathrm{Re}=\rho UL/\mu$, where ρ is the fluid density, U is a characteristic velocity, L is a characteristic length scale, and μ is the dynamic viscosity.

The Laminar Flow interface ( ) describes fluid motion when the Reynolds number is less than approximately 1000, and turbulences are not present. The physics interface solves the Navier-Stokes equations, for incompressible or weakly

compressible flows, where the Mach number (Ma), given by Ma=U/c, where c is the velocity of sound in the fluid, is less than 0.3.

The Creeping Flow interface ( ) approximates the Navier-Stokes equations for the case when the Reynolds number is significantly less than 1. This is often referred to as Stokes flow and is appropriate for use when viscous flow is dominant.

The Phase Transport interface ( )under the Multiphase Flow branch is used to simulate the transport of multiple immiscible phases in free flow. This interface solves for the averaged volume fractions of the phases, and does not track the interface between the different phases.

Another useful tool in these physics interfaces is the ability to describe material properties such as density and viscosity by entering expressions that describe them as a function of other parameters, such as species concentration, pressure, or temperature. Many materials in the material libraries use temperature- and pressure-dependent property values.

Porous Media Flow

The Darcy's Law interface ( ) describes fluid movement through interstices in a porous medium. Because the fluid loses considerable energy to frictional resistance within the pores, flow velocities in porous media are very low. Darcy's Law applies to water moving in an aquifer or stream bank, oil migrating to a well, and even magma rising through the earth to a chamber in a volcano. You can also set up multiple Darcy's Law interfaces to model multiphase flows involving more than one mobile phase.

This physics interface can be used to model low velocity flows, for which the pressure gradient is the major driving force, and the flow is mostly influenced by the frictional resistance within the pores. Its use is within very low flows, or media where the permeability and porosity are very small.

The Fracture Flow interface ( ) is a variant of Darcy's law that defines the flow along interior boundaries representing fractures within a porous (or solid) medium.

The Richards' Equation interface ( ) analyzes flow in variably saturated porous media. With variably saturated flow, hydraulic properties change as fluids move through the medium, filling some pores and draining others. Richards' equation appears similar to the saturated flow equation set out in Darcy's Law, but it is notoriously nonlinear. Nonlinearities arise because the material and hydraulic properties vary from unsaturated to saturated conditions. The analytic formulas of van Genuchten and Brooks and Corey are frequently employed with variably saturated flow modeling. With Darcy's law or Richards' equation, COMSOL Multiphysics solves for pressure and has physics interfaces for pressure head and hydraulic head.

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

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

The Multiphase Flow in Porous Media interface ( ) combines the functionality of the Darcy's Law and Phase Transport in Porous Media interfaces. This multiphysics interface is intended to model flow and transport of multiple immiscible phases in a porous medium.

The Brinkman Equations interface ( ) is used to model compressible flow at moderate speeds, given by a Mach number less than 0.3. You can also choose to model incompressible flow and simplify the equations to be solved. Furthermore, you can select the Stokes-Brinkman flow feature to reduce the equations' dependence on inertial effects, when the Reynolds number is significantly less than one.

The Brinkman Equations interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier-Stokes equation. Consequently, they are well-suited to transitions between slow flow in porous media, governed by Darcy's law, and fast flow in channels described by the Navier-Stokes equations. Interesting uses of the Brinkman to Navier-Stokes coupling include modeling of the hyporheic zone near a river, or the flow of oil through a reservoir into a well. The equations and boundary conditions that describe these types of phenomena are in the Free and Porous Media Flow interface. The Brinkman Equations interface can also add a Forchheimer drag term, which is a viscous drag on the porous matrix proportional to the square of the flow velocity.

The Free and Porous Media Flow interface ( ) is useful for modeling problems where free flow is connected to porous media. It should be noted that if the porous region is large in comparison to the free fluid region, and you are not primarily interested in results in the region of the interface, then you can always couple a Fluid Flow interface to the Darcy's Law interface, to make your overall application computationally cheaper.

The Free and Porous Media Flow interface is used over at least two different domains, a free channel and a porous medium. The physics interface adds

functionality that allows the equations to be optimized according to the flow properties of the relevant domain. For example, you can select the Stokes-Brinkman flow feature to reduce the equations' dependence on inertial effects in the porous domain, or just the Stokes' flow feature to reduce the equations' dependence on inertial effects in the free channel.

As always, the physics interface gives you direct access to defining, with either constants or expressions, the material properties that describe the porous media flow. This includes the density, dynamic viscosity, permeability, and porosity.

Heat Transfer

The Heat Transfer interfaces characterize temperature distributions for geological phenomena and can be freely coupled to other physics interfaces in an application. These physics interfaces apply to systems consisting of solids, fluids, and fluid-solid mixtures, and are able to calculate effective properties for porous media consisting of several fluids, gases and solid components, such as a rock formation with different mineral proportions.

The Heat Transfer in Solids interface ( ) describes, by default, heat transfer by conduction. The physics interface is also able to account for the heat flux due to translation in solids.

The Heat Transfer in Fluids interface ( ) accounts for conduction and convection as the main heat transfer mechanisms. The coupling to the flow field in the convection term may be entered manually, or it may be selected from a list that couples the heat transfer to an existing Fluid Flow interface. The Heat Transfer in Fluids interface can be solved simultaneously with the Laminar Flow interface, or when the flow field has already been calculated and the heat transfer problem is solved afterward, typically for simulations of forced convection.

The Heat Transfer in Porous Media interface ( ) combines the heat conduction and convection in a solid-fluid system. This physics interface provides mixing rules for calculating the effective heat transfer properties, expressions for heat dispersion in porous media, as well as including geothermal heating. Dispersion is caused by the tortuous path of the liquid in the porous medium, which would not be described if only the mean convective term was taken into account. This physics interface may be used for a wide range of porous materials, from porous structures to the simulation of heat transfer in soils and rocks, and also to model heat transfer in fractures.

These features interact seamlessly and can be used in combination in a single application. Surface-to-surface radiation can also be included in the energy equation, although this requires a license for the Heat Transfer Module.

STRUCTURAL MECHANICS

The Poroelasticity interface ( ) combines a transient formulation of Darcy's law with a linear elastic material included in the Solid Mechanics interface. The poroelasticity coupling means that the pore fluid affects the compressibility of the porous medium, as well as changes in volumetric strains will affect the mass transport.

Physics Interface Guide by Space Dimension and Study Type

The table lists the physics interfaces available with this module in addition to those included with the COMSOL basic license.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Chemical Species Transport				
Transport of Diluted Species		tds	all dimensions	stationary; time dependent
Transport of Diluted Species in Porous Media		tds	all dimensions	stationary; time dependent
Transport of Diluted Species in Fractures		dsf	3D, 2D, 2D axisymmetric	stationary; time dependent
Reacting Flow				
Laminar Flow, Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Reacting Flow in Porous Media				
Transport of Diluted Species		rfds	3D, 2D, 2D axisymmetric	stationary; time dependent
Fluid Flow				
Single-Phase Flow				
Creeping Flow		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow[1]		spf	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Phase Transport				
Phase Transport		phtr	3D, 2D, 2D axisymmetric	stationary; time dependent
Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent
Fracture Flow		esff	3D, 2D, 2D axisymmetric	stationary; time dependent
Richards' Equation		dl	all dimensions	stationary; time dependent
Multiphase Flow in Porous Media		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Two-Phase Darcy's Law		tpdl	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport in Porous Media		phtr	3D, 2D, 2D axisymmetric	stationary; time dependent
Heat Transfer				
Heat Transfer in Solids		ht	all dimensions	stationary; time dependent
Heat Transfer in Fluids		ht	all dimensions	stationary; time dependent
Heat Transfer in Solids and Fluids		ht	all dimensions	stationary; time dependent
Heat Transfer in Fractures		htlsh	3D, 2D, 2D axisymmetric	stationary; time dependent; thermal perturbation, frequency domain

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

Aldicarb is a commercial pesticide, used on a variety of crops, including cotton, sugar beet, citrus fruits, potatoes, and beans. People may be exposed to aldicarb primarily through the ingestion of contaminated water and food.

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 chemical compounds are contained in a water pond, treated as a perfectly mixed system.

The second model tracks the detailed distribution of chemicals in the soil as the pesticide leaches out of the pond and is transported by water through the surrounding soil.

Investigating a Perfectly Mixed System

First consider the water pond as a perfectly mixed system. Aldicarb degrades by transformation to the corresponding sulfoxide and sulfone (which are both relatively toxic), and it is detoxified to oximes and nitrile by hydrolysis.

The chain of reactions is illustrated in Figure 2.

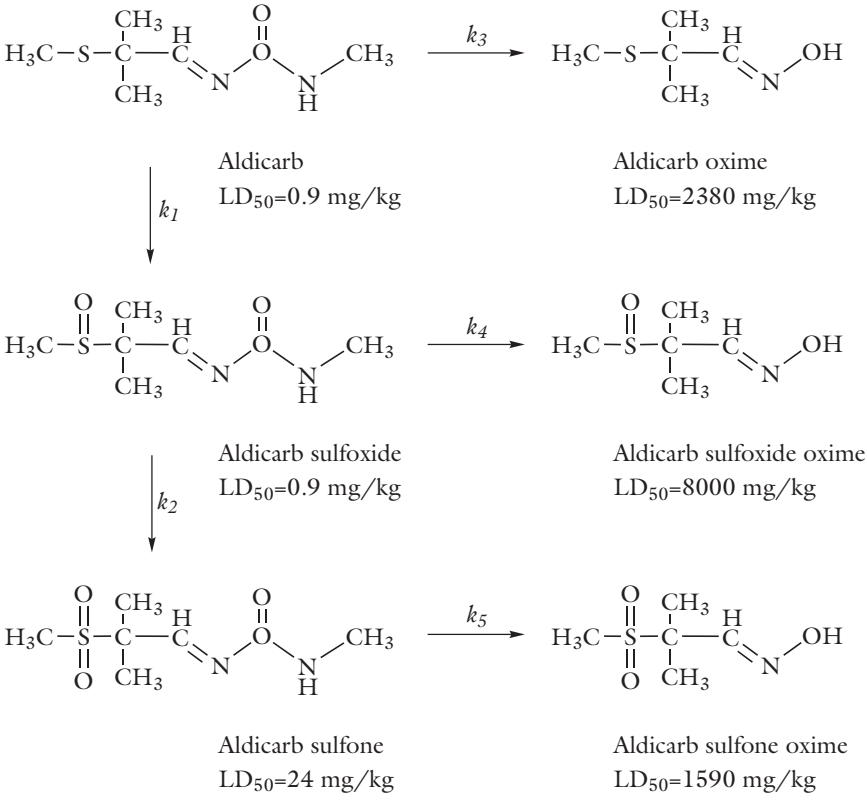

Figure 2: Reaction pathways of aldicarb degradation. The toxicity is indicated by its LD_{50} value (mg/kg), signifying the median lethal dose.

Each of the unimolecular reactions outlined in Figure 2 has a rate expression r_j of the form

$$r_j = k_j c_i \tag{1}$$

In this example, the species concentrations c_j are given in units of mol/m^3, and the rate constants k_j are expressed in 1/day.

The reactions for the chemical species are given by:

- For aldicarb (c_a)

$$\frac{dc_a}{dt} = -r_1 - r_3 = -k_1 c_a - k_3 c_a \tag{2}$$

- For aldicarb sulfoxide (c_{asx})

$$\frac{dc_{\mathrm{asx}}}{dt} = r_1 - r_2 - r_4 = k_1 c_a - k_2 c_{\mathrm{asx}} - k_4 c_{\mathrm{asx}} \tag{3}$$

- For aldicarb sulfone (c_{asn})

$$\frac{dc_{\mathrm{asn}}}{dt} = r_2 - r_5 = k_2 c_{\mathrm{asx}} - k_5 c_{\mathrm{asn}} \tag{4}$$

- For aldicarb oxime (c_{ao})

$$\frac{dc_{\mathrm{ao}}}{dt} = r_3 = k_3 c_{\mathrm{ao}} \tag{5}$$

- For aldicarb sulfoxide oxime (c_{asxo})

$$\frac{dc_{\mathrm{asxo}}}{dt} = r_4 = k_4 c_{\mathrm{asx}} \tag{6}$$

- For aldicarb sulfone oxime (c_{asno})

$$\frac{dc_{\mathrm{asno}}}{dt} = r_5 = k_5 c_{\mathrm{asn}} \tag{7}$$

Solving this set of coupled ODEs provides information on the time scales of the degradation processes in a closed and perfectly mixed system.

Results

The results of the perfectly mixed system, shown in Figure 3, portrait the concentration profiles of aldicarb and its decay by-products and the concentration transients of the three most toxic species — aldicarb, aldicarb sulfoxide, and aldicarb sulfone — as well as their sum (see Figure 2 for LD_{50} values). Only small amounts of aldicarb remain in the pond after 10 days. Considering the summed-up contributions, contamination levels in the water pond remain high even after several months.

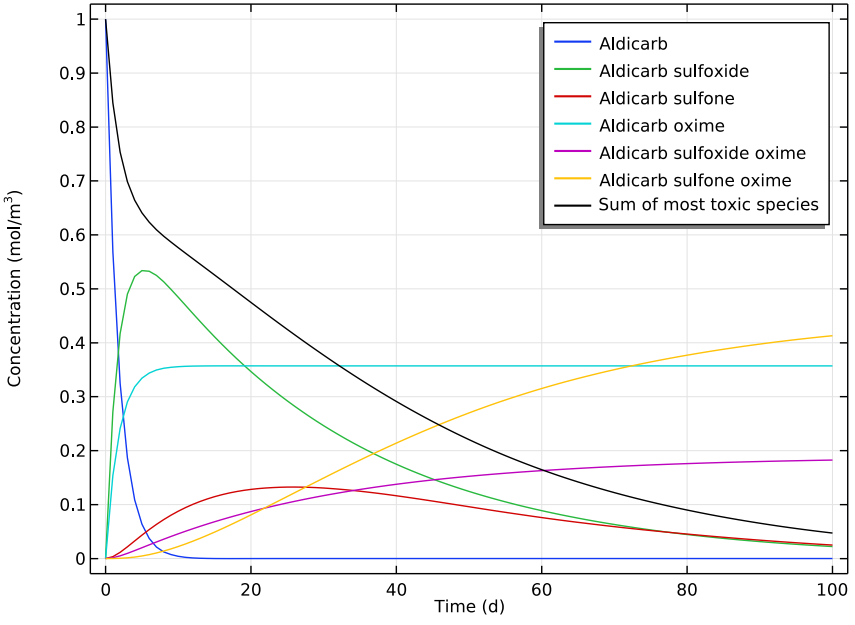

Figure 3: Concentration profiles as reactions occur during a 100 day time period. Concentration transients of the most toxic species, aldicarb (c_a), aldicarb sulfoxide (c_{asx}), aldicarb sulfone (c_{asn}), and the sum of them

Investigating a 2D Model

The results shown in Figure 3 indicate that the concentration of aldicarb, in a pond treated as a perfectly mixed system, decay to less than 1% the initial concentration after 10 days. Consider this time scale as a reference for a more detailed model.

The spatial-dependent model focuses on the concentration of the highly toxic species aldicarb (c_a), aldicarb sulfoxide (c_{asx}), and aldicarb sulfone (c_{asn}). Therefore, you can disregard the mass balances for the hydrogenolysis products (c_{ao}, c_{sxo}, and c_{sno}).

In this more detailed model, you assume that aldicarb moves from the pond into a relatively dry soil. In the soil, the aldicarb decomposes into aldicarb sulfoxide and aldicarb sulfone according to the mechanism illustrated in Figure 2. In addition, the pesticide and its decay by-products are transported by convection, dispersion, adsorption, and volatilization.

Model Geometry

In this application, water is ponded by a ring sitting on the ground. The soil is represented by two layers. The top layer is slightly less permeable than the bottom one, which sits on an almost impervious rock bed. The water moves through the bottom of the ring into the soil. The water level in the ring is known, as is the initial distribution of pressure heads in the soil. There is no flow through the vertical walls or the air-soil surface.

Aldicarb moves with the water from the pond into the soil at a constant concentration. Once in the soil, the chemicals react and adsorb onto soil particles. Aldicarb and the aldicarb sulfone volatilize to the atmosphere. The adsorption, biodegradation, and volatilization proceed is proportional to the aqueous concentrations.

The soil is initially pristine with zero concentration of the involved chemicals. At the ground surface outside the ring, aldicarb and aldicarb sulfone volatilize to the atmosphere.

The left 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. Model the problem with 2D axisymmetry and track the solute transport for 10 days.

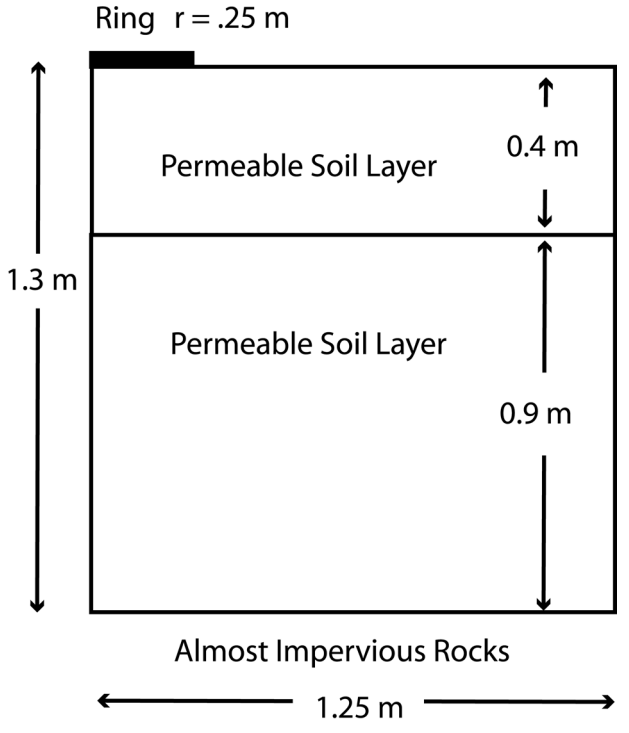

Figure 4: Geometry of the infiltration ring and soil column.

Fluid Flow

Richards' equation governs the saturated-unsaturated flow of water in the soil. The soil pores are connected to the atmosphere, so you can assume that pressure changes in the air do not affect the flow and thus use Richards' equation. Given by Ref. 1, Richards' equation given in pressure head reads

$$(C + \mathrm{Se}S)\frac{\partial H_p}{\partial t} + \nabla \cdot (-K\nabla(H_p + D)) = 0 \tag{8}$$

where C denotes specific moisture capacity (m^{-1}); Se is the effective saturation of the soil (dimensionless); S is a storage coefficient (m^{-1}); H_p is the pressure head (m), which is proportional to the dependent variable, p (Pa); t is time; K equals the hydraulic conductivity (m/s); D is the direction (typically, the z direction) that represents the vertical elevation (m).

To be able to combine boundary conditions and sources with the Darcy's Law and Fracture Flow interfaces, COMSOL Multiphysics converts Richards' equation to SI units and solves for the pressure variable (SI unit: Pa).

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

$$H_p = \frac{p}{\rho g}; \qquad H = H_p + D \tag{9}$$

Also, the soil permeability κ (SI unit: m^{-2}) and hydraulic conductivity K (SI unit: m/s) are related to the fluid viscosity μ (SI unit: Pa·s) and density ρ (SI unit: kg/m^3), and to the acceleration of gravity g (SI unit: m/s^2) by

$$\frac{\kappa}{\mu} = \frac{K}{\rho g} \tag{10}$$

In this model, the specific moisture capacity Cm and the effective saturation Se are taken from the van Genuchten retention model (Ref. 2). For more details see The Richards' Equation interface in the *Subsurface Flow 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.

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_b c_P) + \mathbf{u} \cdot \nabla c + \nabla \cdot (-\theta D_L \nabla c) = \Sigma R_L + \Sigma R_P + S_c \tag{11}$$

The Transport of Diluted Species in Porous Media interface implements the equation above for one or several species. It describes the time rate of change in two terms: c denotes dissolved concentration (mol/m^3) and c_P the mass of adsorbed contaminant per dry unit weight of soil (mg/kg). Further, θ denotes the volume fraction of fluid (dimensionless), and ρ_b is the soil's bulk density (kg/m^3). Because ρ_b amounts to the dried solid mass per bulk volume, the term $\rho_b c_P$ gives the solute mass attached to the soil as the concentration changes with time.

Solute spreading also 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

$$\theta D_{LGii} = \alpha_1 \frac{u_i^2}{|\mathbf{u}|} + \alpha_2 \frac{u_j^2}{|\mathbf{u}|} + \theta \frac{D_m}{\tau_L} + \alpha_v \frac{D_G}{\tau_G} k_G \tag{12}$$

$$\theta D_{LGij} = \theta D_{LGji} = (\alpha_1 - \alpha_2) \frac{u_i u_j}{|\mathbf{u}|} \tag{13}$$

In these equations, $D_{\mathrm{LG}ii}$ are the principal components of the water-air dispersion tensor; $D_{\mathrm{LG}ij}$ and $D_{\mathrm{LG}ji}$ are the cross terms; α is the dispersivity (m) where the subscripts "1" and "2" denote longitudinal and transverse dispersivity; D_{m} and D_{G} (m^2/d) are molecular diffusion coefficients; and τ_{L} and τ_{G} give the tortuosity factors for water and air, respectively.

The three solutes — aldicarb, aldicarb sulfoxide, and aldicarb sulfone — have different decay rates, $R_{\mathrm{L}i}$, partition coefficients, $k_{\mathrm{P}i}$, and volatilization constants, $k_{\mathrm{G}i}$. All the three solutes attach to soil particles, but only aldicarb and aldicarb sulfone volatilize; aldicarb sulfoxide does not.

Results

The following results come from the space- and time-dependent model. Figure 5 shows the fluid flow in soil after 0.3 days (left) and 1 day (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.

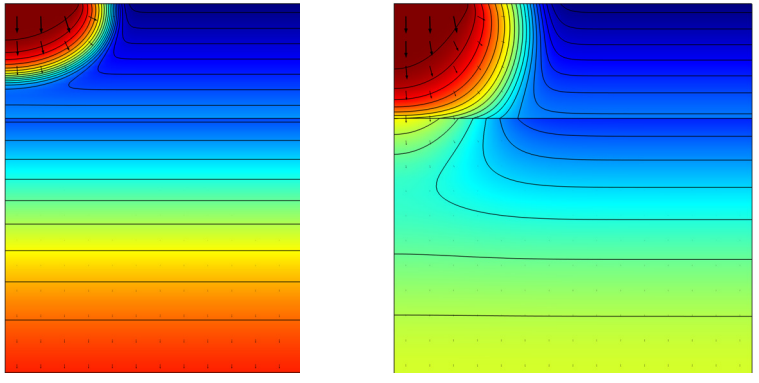

Figure 5: The effective saturation (surface plot), pressure head (contours), and flow velocity (arrows) in a variably saturated soil after 0.3 days (left) and 1 day (right).

Figure 6 through Figure 8 show the concentration distributions 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.

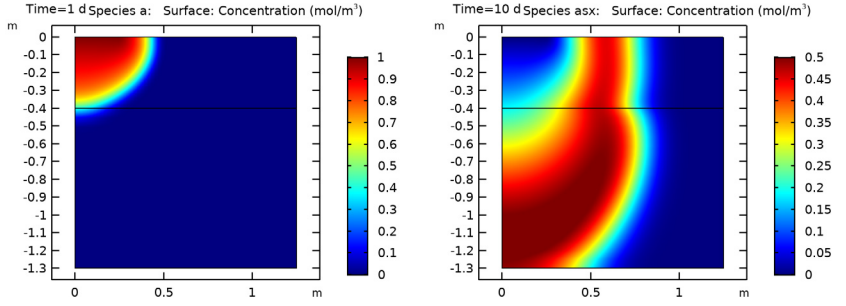

Figure 6: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 1 day.

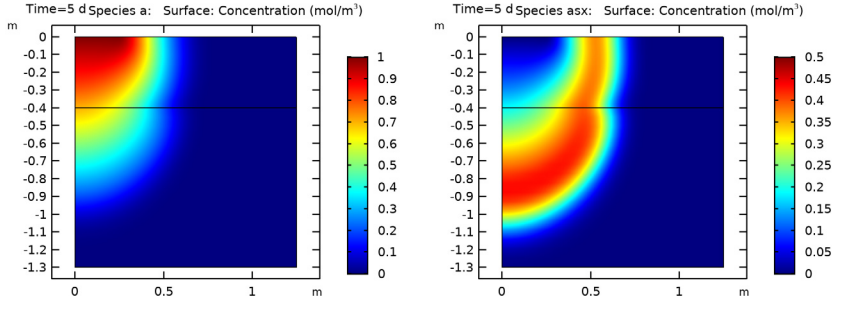

Figure 7: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 5 days.

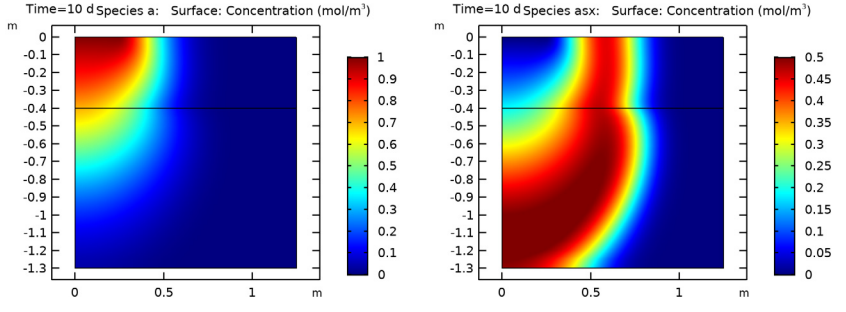

Figure 8: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 10 days.

The distribution of aldicarb has clearly reached steady-state conditions after 10 days, a time frame that was also predicted by the ideal reactor model (see Figure 2). 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.

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1. J. Bear, *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 Wizard

Note: These instructions are for the user interface on Windows but apply, with minor differences, also to Linux and Mac.

1. To start the software, double-click the COMSOL icon on the desktop. When the software opens, you can choose to use the Model Wizard to create a new COMSOL model or Blank Model to create one manually. For this tutorial, click the Model Wizard button.

   If COMSOL is already open, you can start the Model Wizard by selecting New from the File menu and then click Model Wizard .

   The Model Wizard guides you through the first steps of setting up a model. The next window lets you select the dimension of the modeling space.

2. In the Select Space Dimension window click 2D Axisymmetric .
3. In the Select Physics tree, under Mathematics>ODE and DAE Interfaces, double-click Global ODEs and DAEs (ge) to add it to the Added physics interfaces list. You can also click Add or right-click and choose Add Physics .
4. Click Study . In the Select Study window under General Studies, click Time Dependent .
5. Click Done .

Reactions

The reaction mechanism illustrated in Figure 2 translates into the mass balance equations for aldicarb, aldicarb sulfoxide, aldicarb sulfone, aldicarb oxime, aldicarb sulfoxide oxime, and aldicarb sulfone oxime. Solving this set of coupled ODEs provides information on the time scales of the degradation processes.

First treat the aldicarb decomposition kinetics in the water pond as a perfectly mixed system. Start by importing a set of global parameters defining the rate constants k_j expressed in 1/day, and the reactions for the chemical species given by Equation 2 through Equation 7.

Note: The location of the files used in this exercise varies based on the installation. For example, if the installation is on your hard drive, the file path might be similar to

`C:\Program Files\COMSOL\COMSOL55\Multiphysics\applications\`.

Parameters

1 On the Home toolbar click Parameters P_i. You can also right-click Global Definitions in the Model Builder and select Parameters P_i.

Note: On Linux and Mac, the Home toolbar refers to the specific set of controls near the top of the Desktop.

2 In the Settings window for Parameters click the Load from File button.

3 Browse to the file `pesticide_transport_parameters_1.txt` in the Application Libraries folder on your computer, Subsurface_Flow_Module\Solute_Transport. Double-click to add or click Open.

The rate constants are added to the table.

Parameters

Name	Expression	Value	Description
k_1	0.36[1/d]	4.1667E-6 1/s	Rate constant, reaction 1
k_2	0.024[1/d]	2.7778E-7 1/s	Rate constant, reaction 2
k_3	0.2[1/d]	2.3148E-6 1/s	Rate constant, reaction 3
k_4	0.01[1/d]	1.1574E-7 1/s	Rate constant, reaction 4
k_5	0.0524[1/d]	6.0648E-7 1/s	Rate constant, reaction 5

Reactions

1 In the Model Builder, under Global ODEs and DAEs, click Global Equations $\frac{d}{dt}$.

2 In the Settings window for Global Equations click the Load from File button.

3 Browse to the file `pesticide_transport_reactions.txt` in the Application Libraries folder on your computer, Subsurface_Flow_Module\Solute_Transport. Double-click to add or click Open.

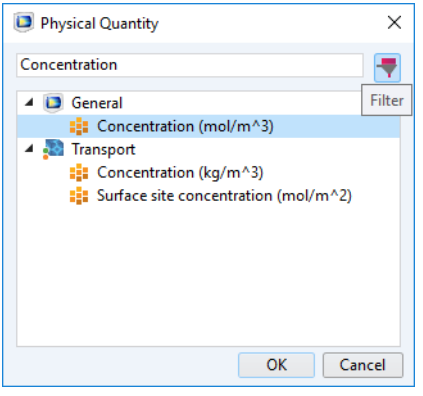
The reactions are added to the table.

Global Equations

$f(u,u_t,u_{tt},t)=0,\ u(t_0)=u_0,\ u_t(t_0)=u_{t0}$

Name	f(u,ut,utt,t) (mol/(m^3*s))	Init	Init	Description
cpm_a	cpm_at+k_1*cpm_a+k_3*cpm_a	1	0	Aldicarb
cpm_asx	cpm_asxt-k_1*cpm_a+k_2*cpm_asx+k_4*cpm_asx	0	0	Aldicarb sulfoxide
cpm_asn	cpm_asnt-k_2*cpm_asx+k_5*cpm_asn	0	0	Aldicarb sulfone
cpm_ao	cpm_aot-k_3*cpm_a	0	0	Aldicarb oxime
cpm_asxo	cpm_asxot-k_4*cpm_asx	0	0	Aldicarb sulfoxide oxime
cpm_asno	cpm_asnot-k_5*cpm_asn	0	0	Aldicarb sulfone oxime

Locate the Units section and click the Select dependent variable quantity button. In the Physical Quantity dialog box type `Concentration` and click the Filter button. Choose Concentration (mol/m^3) and click OK. Repeat the same procedure for the Source term quantity section, and choose Reaction rate (mol/(m^3*s)) as unit.

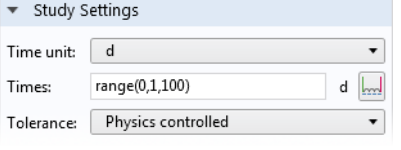


The chemical reactions (given by Equation 2 through Equation 7) are slightly modified. All the terms are moved to the left-hand side. Also note that the initial values are zero for all the concentrations, except for aldicarb.

Study 1

Time Dependent

1. In the Model Builder expand the Study 1 node and click Step 1: Time Dependent.
2. Go to the Settings window for Time Dependent. Under Study Setting, select `d` (for days) from the Time unit list.
3. In the Times text field enter `range(0,1,100)`.



4 On the Home toolbar click Compute .

You can also right-click Study 1 in the Model Builder and select Compute .

Results — Decomposition Kinetics

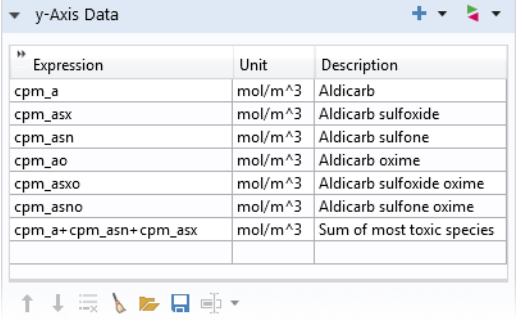
Follow these steps to generate result plots for the decomposition kinetics of aldicarb occurring in a water pond treated as a closed and perfectly mixed system.

1D Plot Group 1

1 Under Results click the 1D Plot Group 1 node . In the Graphics window the Global plot is shows the concentration profile for the six species. To plot the concentration of the most toxic species, as in Figure 3, proceed as follows:

2 Expand the 1D Plot Group 1 node and click Global 1 .

3 In the Settings window for Global under y-Axis Data, add the expression for the total concentration of the most toxic species, `cpm_a+cpm_asn+cpm_asx`, and write Sum of most toxic species in the Description box.



Expression	Unit	Description
cpm_a	mol/m^3	Aldicarb
cpm_asx	mol/m^3	Aldicarb sulfoxide
cpm_asn	mol/m^3	Aldicarb sulfone
cpm_ao	mol/m^3	Aldicarb oxime
cpm_asxo	mol/m^3	Aldicarb sulfoxide oxime
cpm_asno	mol/m^3	Aldicarb sulfone oxime
cpm_a+cpm_asn+cpm_asx	mol/m^3	Sum of most toxic species

4 Click Plot .

The Global plot in Figure 3 is displayed in the Graphics window.

2D Component

Now solve the space and time-dependent transport and reaction of solutes.

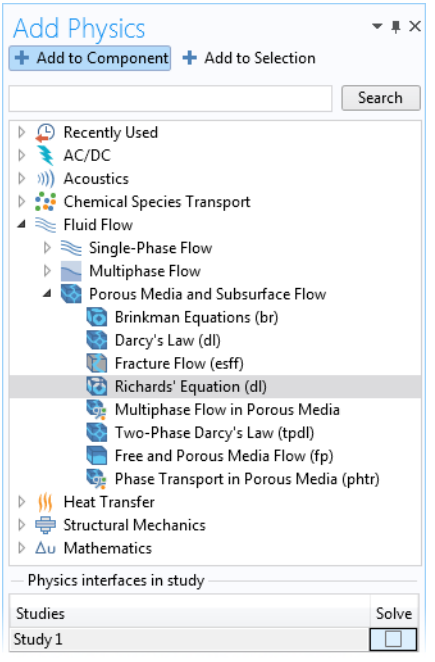
1 On the Home toolbar click Add Physics .

You can also right-click Component 1 in the Model Builder and choose Add Physics .

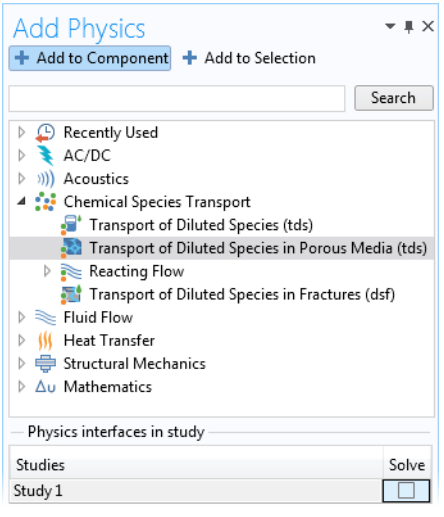
2 Go to the Add Physics window. In the Physics tree, under Fluid Flow>Porous Media and Subsurface Flow, select Richards' Equations (dl) .

3 Find the Physics interfaces in study section immediately below the tree (scroll down if necessary), and deactivate this physics interface in Study 1.

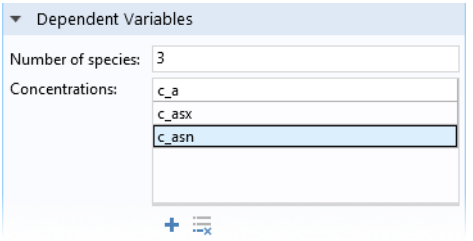
4 Click Add to Component.



5 In the Physics tree, under Chemical Species Transport, click Transport of Diluted Species in Porous Media (tds) . Find the Physics interfaces in study section and click to deactivate this physics interface in Study 1.



6 Click to expand the Dependent variables section. In the Number of species text field, type 3. Change the default names to `c_a`, `c_asx` and `c_asn`.



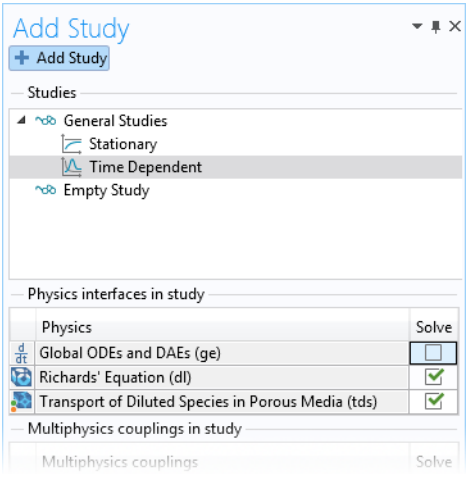
7 Click the Add to Component button ✚.

8 On the Home toolbar click Add Study.

9 Go to the Add Study window and find the Studies section. In the tree under General Studies select Time Dependent.

10 Go to the Physics interfaces in study section and deactivate ☐ the Global ODEs and DAEs (ge) $\frac{d}{dt}$ physics.

11 Click the Add Study button ✚.



Parameters and Variables

Import a set of global parameters defining the material parameters for Richards' Equation and Solute Transport, including the fluid density, viscosity, porosity, storage coefficients, hydraulic conductivity, dispersivity, and so forth.

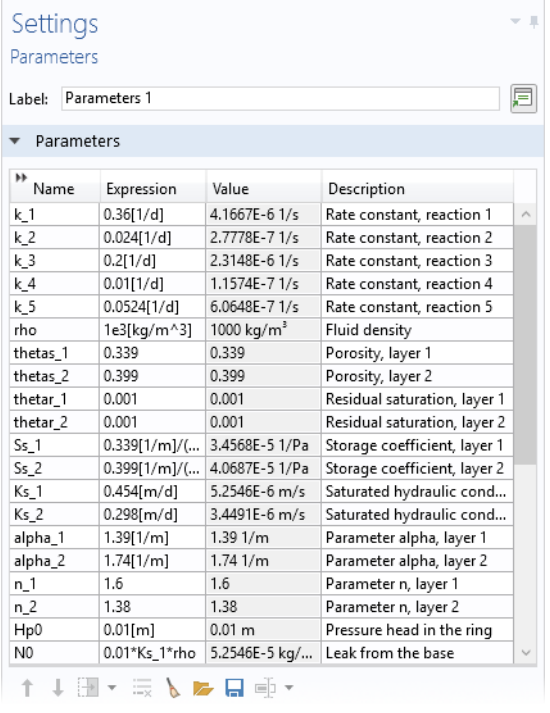
Then, import a set of variables specifying the rate expressions given by Equation 2 through Equation 7.

Note: The location of the files used in this exercise varies based on the installation. For example, if the installation is on your hard drive, the file path might be similar to `C:\Program Files\COMSOL\COMSOL55\Multiphysics\applications\`.

Parameters

1. In the Model Builder expand Global Definitions and click Parameters .
2. In the Settings window for Parameters click the Load from File button .
3. Browse to the file `pesticide_transport_parameters_2.txt` in the Application Libraries folder on your computer, Subsurface_Flow_Module\Solute_Transport. Double-click to add or click Open.

The parameters are added to the table.



Name	Expression	Value	Description
k_1	0.36[1/d]	4.1667E-6 1/s	Rate constant, reaction 1
k_2	0.024[1/d]	2.7778E-7 1/s	Rate constant, reaction 2
k_3	0.2[1/d]	2.3148E-6 1/s	Rate constant, reaction 3
k_4	0.01[1/d]	1.1574E-7 1/s	Rate constant, reaction 4
k_5	0.0524[1/d]	6.0648E-7 1/s	Rate constant, reaction 5
rho	1e3[kg/m^3]	1000 kg/m³	Fluid density
thetas_1	0.339	0.339	Porosity, layer 1
thetas_2	0.399	0.399	Porosity, layer 2
thetar_1	0.001	0.001	Residual saturation, layer 1
thetar_2	0.001	0.001	Residual saturation, layer 2
Ss_1	0.339[1/m]/(...	3.4568E-5 1/Pa	Storage coefficient, layer 1
Ss_2	0.399[1/m]/(...	4.0687E-5 1/Pa	Storage coefficient, layer 2
Ks_1	0.454[m/d]	5.2546E-6 m/s	Saturated hydraulic cond...
Ks_2	0.298[m/d]	3.4491E-6 m/s	Saturated hydraulic cond...
alpha_1	1.39[1/m]	1.39 1/m	Parameter alpha, layer 1
alpha_2	1.74[1/m]	1.74 1/m	Parameter alpha, layer 2
n_1	1.6	1.6	Parameter n, layer 1
n_2	1.38	1.38	Parameter n, layer 2
Hp0	0.01[m]	0.01 m	Pressure head in the ring
N0	0.01*Ks_1*rho	5.2546E-5 kg/...	Leak from the base

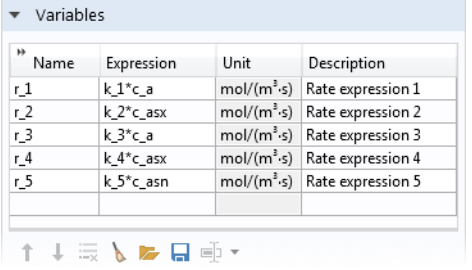
Variables 1

1 In the Model Builder under Component 1, right-click Definitions and select Variables .

2 In the Settings window under Variables, click the Load from File button .

3 Browse to the file `pesticide_transport_variables.txt` in the Application Libraries folder on your computer, Subsurface_Flow_Module\Solute_Transport. Double-click to add or click Open.

The rate expressions are added to the table.



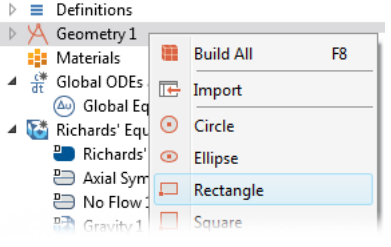
Geometry

The modeling domain is made up of the two permeable soil layers, each of which is represented by a rectangular domain in 2D axisymmetry. Add an additional layer to the right boundary to define an Infinite Element domain.

1 In the Model Builder right-click Geometry 1 and add a Rectangle . This represents the lower layer of soil.

2 In the Settings window for Rectangle locate the Size and Shape section.
- In the Width text field type `1.5`.
- In the Height text field type `0.9`.

3 Under Position in the z text field, type `-1.3`.

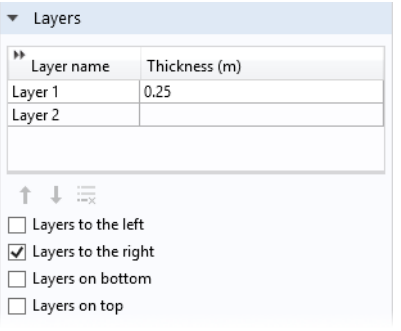


4 Expand the Layers section, select the Layers to the right check box and type `0.25` in the Thickness text field.

5 Right-click Geometry 1 and add another Rectangle . This represents the upper layer of soil.

6 In the Settings window for Rectangle locate the Size and Shape section.

- In the Width text field type `1.5`.
- In the Height text field type `0.4`.



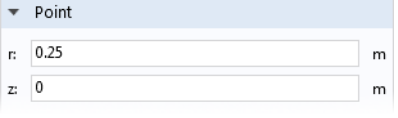
7 Under Position in the z text field, enter `-0.4`.

8 Expand the Layers section, type `0.25` in the Thickness text field, and select the Layers to the right check box.

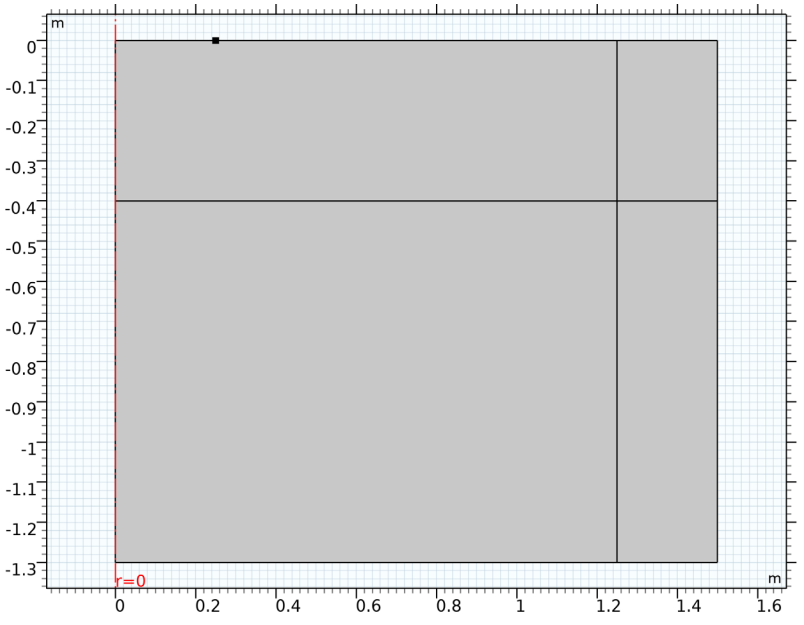
These additional layers to the right of the geometry will be used to define Infinite Element Domains. To finish the model geometry, add a point on the top boundary to make the pond's outer rim.

1 Right-click Geometry 1 and add a Point .

2 In the Settings window for Point locate the Point section. In the r text field, type `0.25`.



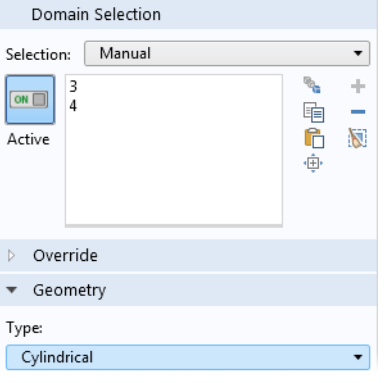
3 Click Build All Objects .



Infinite Element Domain 1

1 In the Model Builder under Component 1, right-click Definitions and select Infinite Element Domain . Select domains 3 and 4 only.

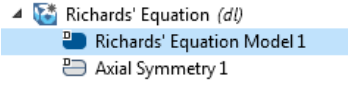
2 In the Settings window for Infinite Element Domain, locate the Geometry section and choose Cylindrical.



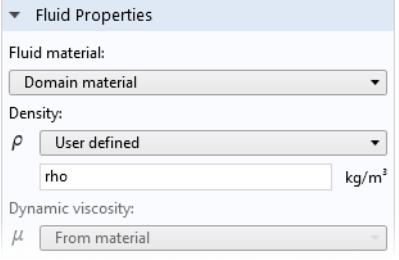
Begin by specifying the properties for the bottom soil layer in the default Richards' Equation Model node, then duplicate this node and modify the domain selection and properties to match the top layer.

Richards' Equation Model 1

1 In the Model Builder Under the Richards' Equation interface, click the Richards' Equation Model 1 node.

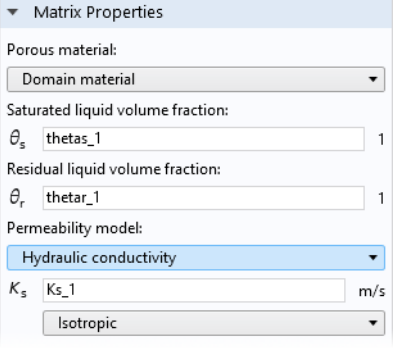


2 Under the Fluid Properties section, select User defined from the Density list. In the ρ text field, enter `rho`.



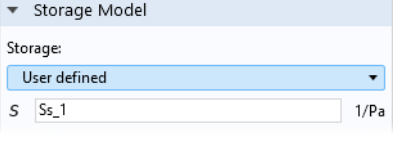
3 Under Matrix Properties:

- In the θ_s text field, enter `thetas_1`.
- In the θ_r text field, enter `thetar_1`.
- From the Permeability Model list, select Hydraulic conductivity. In the K_s text field, enter `Ks_1`.



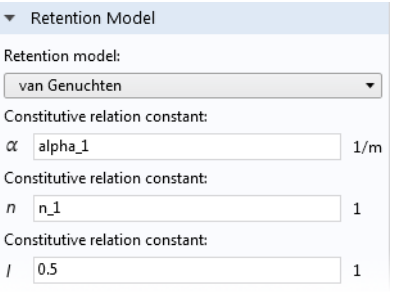
4 Under Storage Model:

- From the Storage list, select User defined.
- In the Storage text field, enter `Ss_1`.



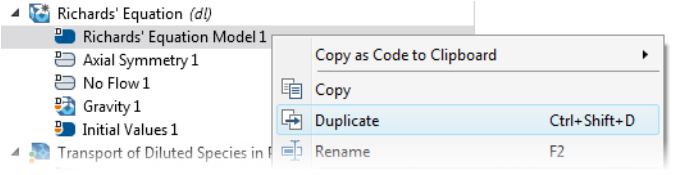
5 Under Retention Model:

- Use the default van Genuchten model in the Retention model list.
- In the α text field, enter `alpha_1`.
- In the n text field, enter `n_1`.
- Leave the default value `0.5` in the l text field.

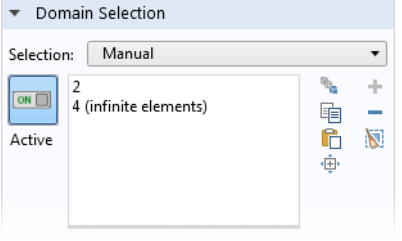


Richards' Equation Model 2

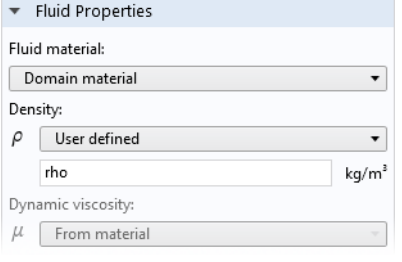
1 In the Model Builder right-click Richards' Equation Model 1. Select Duplicate .



2 In the Settings window for Richards' Equation Model 2 verify that the Domain Selection consists of domains 2 and 4.



3 Under Fluid Properties, keep User defined in the Fluid material list and type `rho` in the ρ text field.



4 Under Matrix Properties:

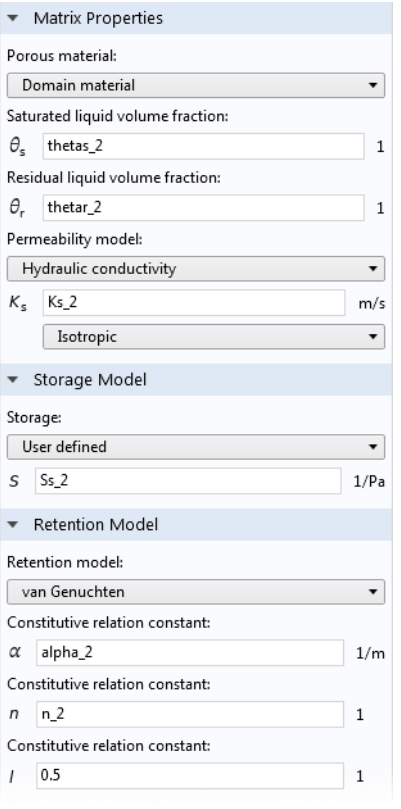
- In the θ_s text field, enter `thetas_2`.
- In the θ_r text field, enter `thetar_2`.
- From the Permeability Model list, keep Hydraulic conductivity. In the K_s text field, enter `Ks_2`.

5 Under Storage Model:

- Keep User defined in the Storage list.
- In the Storage text field, enter `Ss_2`.

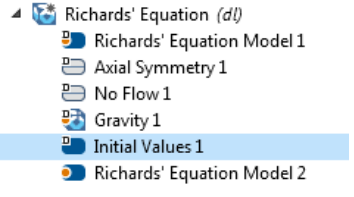
6 Under Retention Model:

- Keep the default van Genuchten model in the Retention model list.
- In the α text field, enter `alpha_2`.
- In the n text field, enter `n_2`.
- Keep the default value `0.5` in the l field.



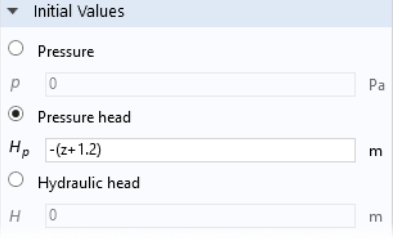
Initial Values 1

1 Select Initial Values 1 under Richards' Equation (dl).



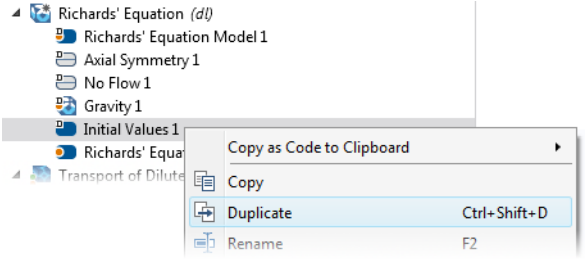
2 Locate the Initial Values section, and click the Pressure head button.

3 In the H_p text field, enter `-(z+1.2)` to set the water table to 1.2 m below the surface.



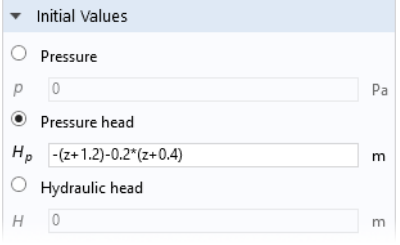
Initial Values 2

1 Under Richards' Equation (dl) right-click Initial Values 1. Select Duplicate .



2 In the Settings window for Initial Values 2 under Domain Selection, add domains 2 and 4.

3 In the Settings window for locate the Initial Values section. In the H_p text field, enter `-(z+1.2)-0.2*(z+0.4)`.



Pressure Head 1

1 In the Model Builder click Richards' Equation (dl) . On the Physics toolbar click Boundaries and select Pressure Head.

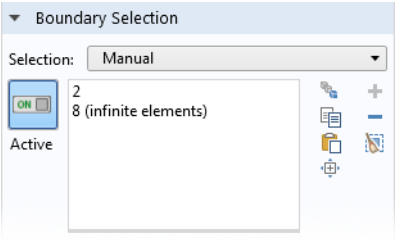
2 In the Boundary Selection window, select Boundary 5 only.

3 Under Pressure Head, enter `Hp0` in the H_{p0} text field.

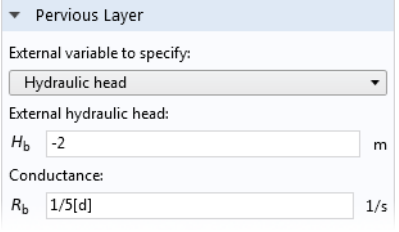
Pervious Layer 1

1 On the Physics toolbar click Boundaries and select Pervious Layer.

2 In the Boundary Selection window, select Boundaries 2 and 8 only.

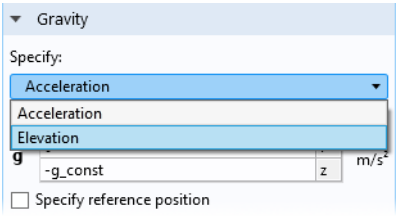


3 Find the Pervious Layer section, under External hydraulic head enter `-2` in the H_b text field, and under Conductance enter `1/5[d]` in the R_b text field.



Gravity 1

1 Gravity 1 under Richards' Equation (dl).



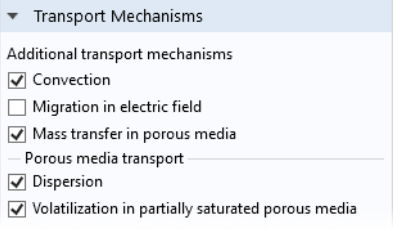
2 Locate the Gravity section, and choose Elevation from the list.

Transport of Diluted Species in Porous Media

The Transport of Diluted Species in Porous Media node will use some of the variables solved in the Richards' Equation interface. Darcy's velocity, saturated volume fraction, and so forth, are denoted by the `dl` prefix. Other variables and material parameters are taken from the imported files.

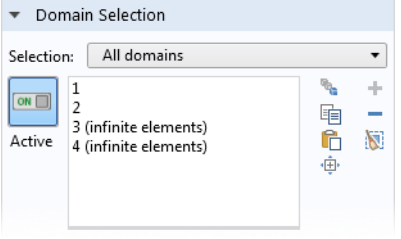
1 In the Model Builder under Component 1, click Transport of Diluted Species in Porous Media (tds) . In the Settings window locate the Transport Mechanisms section. Convection is selected by default.

- Select the Mass transfer in porous media check box.
- Under Porous media transport, select the Dispersion check box.
- Select the Volatilization in partially saturated porous media check box.



2 On the Physics toolbar click Domains and select Partially Saturated Porous Media .

3 In the Settings window for Partially Saturated Porous Media, under Domain Selection select All domains from the Selection list.

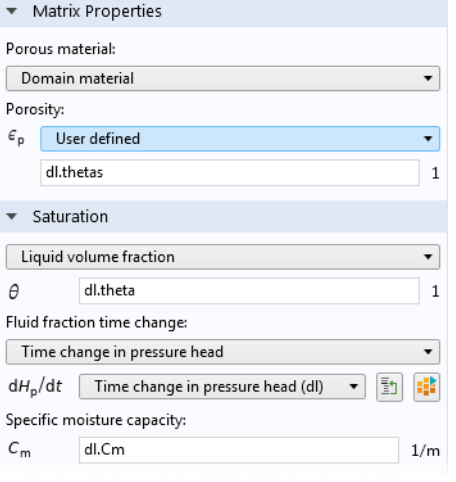


4 Under Matrix Properties

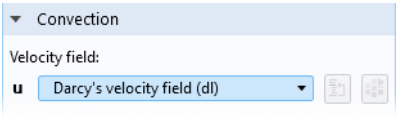
- In the ε_p list choose User defined, then enter `dl.thetas` in the text field.

5 Under Saturation

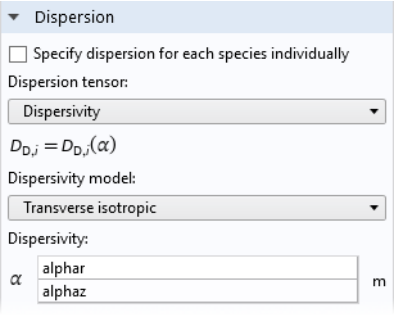
- In the list change from Saturation to Liquid volume fraction, then enter `dl.theta` in the θ text field.
- From the Fluid fraction time change list, select Time change in pressure head. In the dH_p/dt list, select Time change in pressure head (dl).
- Under Specify moisture capacity, enter `dl.Cm` in the C_m text field.



6 Couple the mass transport to the fluid flow. Locate the Convection section, select Darcy's velocity field (dl) from the **u** list.

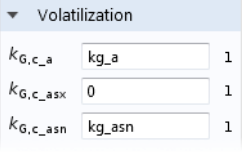


7 Click to expand the Dispersion section. For the Dispersion tensor list, select Dispersivity. For the Dispersivity model list, select Transverse isotropic. Enter `alphar` and `alphaz`.



8 Click to expand the Volatilization section.

- In the $k_{G,ca}$ text field, enter `kg_a`.
- In the $k_{G,casx}$ text field, keep the default value `0`.
- In the $k_{G,casn}$ text field, enter `kg_asn`.



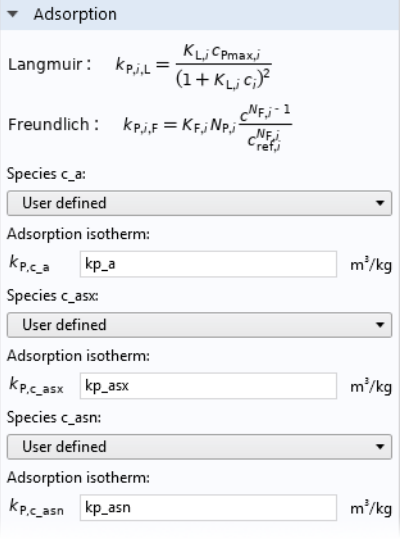
Adsorption 1

1 Under Transport of Diluted Species in Porous Media (tds), right-click Partially Saturated Porous Media 1 and choose Adsorption.

2 In the Matrix Properties section, from tthe ρ list choose User defined, then enter `rhob` in the text field.

3 Click to expand the Adsorption section.

- For the Species c_a list, select User defined. Under User-defined isotherm, in the $k_{P,ca}$ text field, enter `kp_a`.
- For the Species c_asx list, select User defined. Under User-defined isotherm, in the $k_{P,casx}$ text field, enter `kp_asx`.
- For the Species c_asn list, select User defined. Under User-defined isotherm, in the $k_{P,casn}$ text field, enter `kp_asn`.



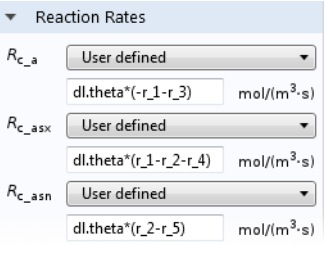
Reactions 1

1 On the Physics toolbar click Domains and select Reactions .

2 In the Settings window for Reactions locate the Domain Selection section. From the Selection list, choose All domains.

3 In the Reaction Rates section:

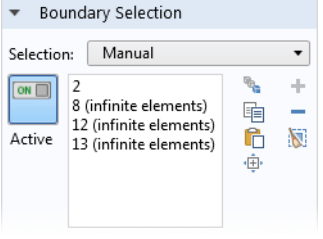
- In the R_{c_a} text field, enter `dl.theta*(-r_1-r_3)`.
- In the R_{c_asx} text field, enter `dl.theta*(r_1-r_2-r_4)`.
- In the R_{c_asn} text field, enter `dl.theta*(r_2-r_5)`.



Outflow 1

1 On the Physics toolbar click Boundaries and select Outflow .

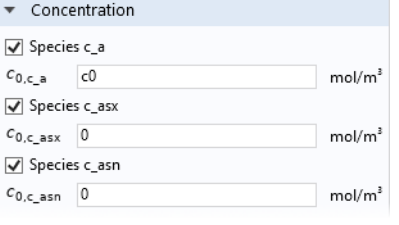
2 In the Settings window for Outflow locate the Boundary Selection section. From the Selection list, select Manual and choose Boundaries 2, 8, 12 and 13 only.



Concentration 1

1 On the Physics toolbar click Boundaries and select Concentration .

2 In the Settings window for Concentration locate the Boundary Selection section. From the Selection list, select Manual and choose Boundary 5 only.



3 In the Concentration section select all three check boxes.

- In the c_{0,c_a} text field, enter `c0`.
- In the c_{0,c_asx} text field, keep the default `0`.
- In the c_{0,c_asn} text field, keep the default `0`.

No Flow Boundary Volatilization 1b

1 On the Physics toolbar click Boundaries and select Volatilization.

2 In the Settings window for Volatilization locate the Boundary Selection section. From the Selection list, select Manual and choose Boundaries 6 and 11 only.

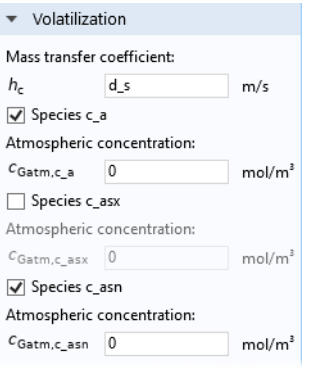
3 In the Volatilization section, under Layer thickness, enter `d_s` in the d_s text field.

4 Select the Species c_a check box.

- In the $c_{Gatm,ca}$ text field, keep the default value `0`.

5 Select the Species c_asn check box.

- In the $c_{Gatm,casn}$ text field, keep the default value `0`.



Mesh

Using a Mapped mesh is a good idea for this geometry.

1 In the Model Builder click Mesh 1. In the Settings window for Size locate the Element Size section. From the Predefined list, choose Finer.

2 In the Model Builder right-click Mesh 1 and select Mapped 1. Right-click Mapped 1 and select Size.

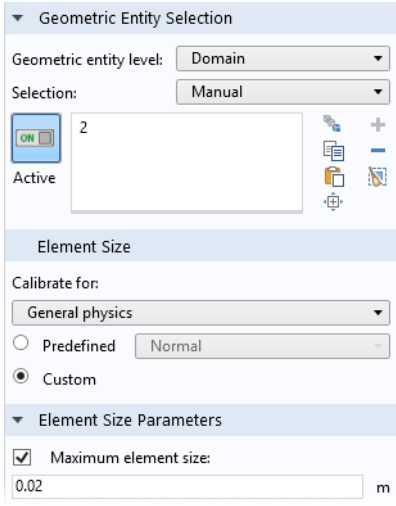
3 In the Settings window for Size 1, locate the Geometric Entity Selection section. From the Selection list, select Manual and choose Domain 2 only.

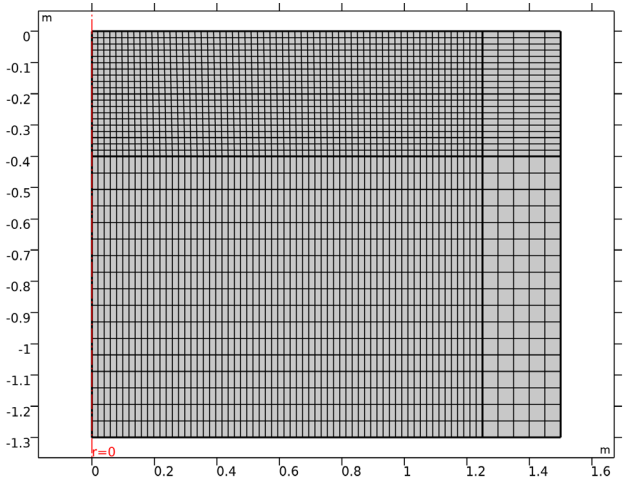
4 In the Element Size section click the Custom button.

5 Locate the Element Size Parameters section. Select the Maximum element size check box.

6 In the associated text field, type `0.02`.

7 Click Build All .





Study 2

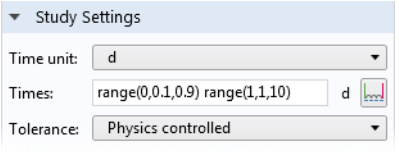
Step 1: Time Dependent

1 In the Model Builder expand the Study 2 node and click Step 1: Time Dependent .

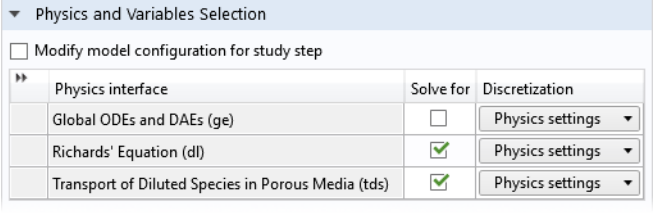
2 Go to the Study Settings section and select d from the Time unit list. This allows plotting the results versus time in days.

3 In the Times text field enter

```
range(0,0.1,0.9) range(1,1,10).
```



4 Locate the Physics and Variables Selection section. In the table, the check mark in the Solve for column indicates which physics interface will be solved in the Study 2. The ODEs are already solved in the Study 1.



5 On the Home toolbar click Compute . You can also right-click Study 2 in the Model Builder, and select Compute .

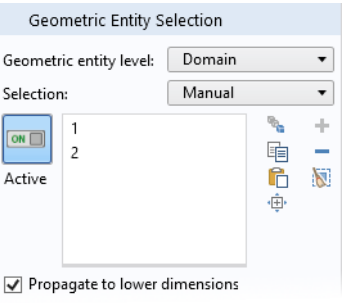
Results

Flownet, pressure and concentration plots are created by default. Pressure and concentration are also visualized on the revolved 3D geometry. Focus on the region close to the pond. Hide the infinite element domains from the plots with the following steps.

Study 2 / Solution 2 (sol2)

1 In the Model Builder expand the Data Sets node under Results, right-click Study2/ Solution 2, and select Selection.

2 In the Settings window locate the Geometric Entity Selection section. From the Geometric entity level list, choose Domain. Select Domain 1 and 2 only. This will remove the Infinite Element domains from the plot groups.



The first default plot group contains a surface plot of the pressure distribution. Modify it to show the effective saturation, pressure head, and velocity field at different times.

Pressure (dl)

1 In the Model Builder under Results, expand the Pressure (dl) node and click Surface.

2 In the Settings window for Surface locate the Expression section and click Replace Expression. From the menu, choose Richards' Equation>Effective saturation (dl.Se), or enter `dl.Se` in the Expression text field.

3 In the Model Builder click Pressure (dl). In the Settings window for 2D Plot Group, type `Effective saturation` in the Label text field.

4 In the Surface setting window locate the Coloring and Style section and clear the Color legend check box. Click the Zoom Extents button on the Graphics toolbar.

5 In the Model Builder under Results click Effective saturation. On the Effective saturation toolbar click Contour.

6 In the Settings window for Contour click Replace Expression. From the menu, choose Component 1>Richards' Equation>Pressure head (dl.Hp), or enter `dl.Hp` in the Expression text field.

7 Locate the Coloring and Style section.

- From the Coloring list, choose Uniform.
- From the Color list, choose Black and clear the Color legend check box.

8 Click to expand the Quality section. From the Resolution list, choose Finer.

9 Click the Effective saturation node. On the Effective saturation toolbar click Arrow Surface. In the Settings window for Arrow Surface, locate the Expression section and enter `dl.u` and `dl.w` to plot Darcy's velocity field.

10 In the Settings window for Arrow Surface locate the Coloring and Style section and from the Color list, choose Black.

11 Click the Effective saturation node. In the Settings window for 2D Plot Group locate the Data section and from the Time list choose 0.3 day.

12 Click the Plot button . Compare the plot in the Graphics window with that in the left panel of Figure 5.

13 Click Effective saturation . In the Settings window for 2D Plot Group locate the Data section and from the Time list choose 1 day.

14 Click the Plot button . Compare the plot in the Graphics window with that in the right panel of Figure 5

Concentration, aldicarb

1 In the Model Builder under Results, expand the Concentration (tds) node, and click Surface .

2 In the Settings window for Surface locate the Range section and select the Manual color range check box. In the Minimum text field type `0` and in the Maximum text field type `1`. This gives a single color range for all the concentration plots and remove spurious negative concentration levels.

3 Click the Plot button and then click the Zoom Extents button on the Graphics toolbar.

The default plot shows the solute concentration at the last resolved time, which is 10 days. Follow the steps below to reproduce the plots shown in Figure 6 through Figure 8.

4 In the Model Builder under Results click Concentration (tds) .

5 In the Settings window for 2D Plot Group locate the Data section, and from the Time list choose 5 days. Click Plot .

6 To plot the concentration after 1 day, select 1 from the Time list.

7 Click Concentration (tds) . In the Settings window for 2D Plot Group, type `Concentration, aldicarb` in the Label text field.

Concentration, aldicarb sulfoxide

1 Under Results right-click Concentration, aldicarb , and choose Duplicate .

2 Expand Concentration, aldicarb 1 and click Surface 1.1 . In the Settings window for 2D Plot Group, type `Concentration, aldicarb sulfoxide` in the Label text field.

3 In the Settings window for Surface click Replace Expression . From the menu, choose Component 1>Transport of Diluted Species in Porous

Media>Species c_asx>Concentration (c_asx), or enter `c_asx` in the Expression text field. This plots the aldicarb sulfoxide concentration.

4 Expand the Range section. In the Maximum text field type `0.5`.

Because the maximum concentration for aldicarb sulfoxide is lower than aldicarb, this setting makes better use of the color range.

5 Click Plot .

6 To reproduce the plots shown in Figure 6 through Figure 8, click Concentration, aldicarb sulfoxide . In the Settings window for 2D Plot Group locate the Data section, and from the Time list choose 1, 5 and 10 days. Click Plot .

You can also visualize the concentration distributions through time. In the Model Builder, under Export , you can generate animations in GIF, Flash, and AVI format.

Alternatively, add animations by click the Animation button on the Results toolbar.