Subsurface Flow Module

COMSOL

Introduction to the Subsurface Flow Module

Version: COMSOL 6.2

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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.
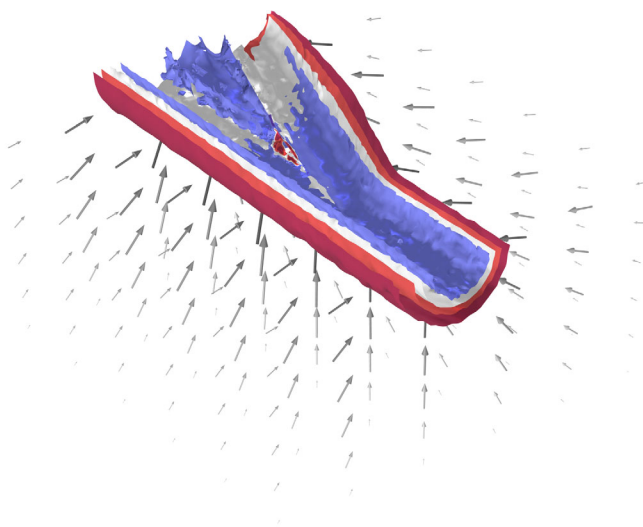
Isosurface plot of the fail function and Darcy velocity field (arrows) calculated from a poroelastic model for the branching junction in a multilateral well.

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 accounts 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.

- Chemical Species Transport
  - Transport of Diluted Species (tds)
  - Transport of Diluted Species in Porous Media (tds)
  - Reacting Flow
  - Reacting Flow in Porous Media
  - Transport of Diluted Species in Fractures (dsf)
- Fluid Flow
  - Single-Phase Flow
    - Creeping Flow (spf)
    - Laminar Flow (spf)
  - Multiphase Flow
    - Phase Transport
      - Phase Transport (phtr)
      - Phase Transport in Porous Media (phtr)
      - Phase Transport in Free and Porous Media Flow (phtr)
  - Porous Media and Subsurface Flow
    - Brinkman Equations (br)
    - Darcy's Law (dl)
    - Fracture Flow (ff)
    - Richards' Equation (dl)
    - Multiphase Flow in Porous Media
    - Two-Phase Darcy's Law (tpdl)
    - Free and Porous Media Flow, Brinkman (fp)
    - Free and Porous Media Flow, Darcy
  - Nonisothermal Flow
    - Laminar Flow
    - Brinkman Equations
  - Fluid–Structure Interaction
  - Shallow Water Equations
- Heat Transfer
  - Heat Transfer in Solids (ht)
  - Heat Transfer in Fluids (ht)
  - Heat Transfer in Solids and Fluids (ht)
  - Conjugate Heat Transfer
  - Electromagnetic Heating
  - Thin Structures
    - Heat Transfer in Fractures (htlsh)
  - Porous Media
- Structural Mechanics
  - Solid Mechanics (solid)
  - Fluid–Structure Interaction
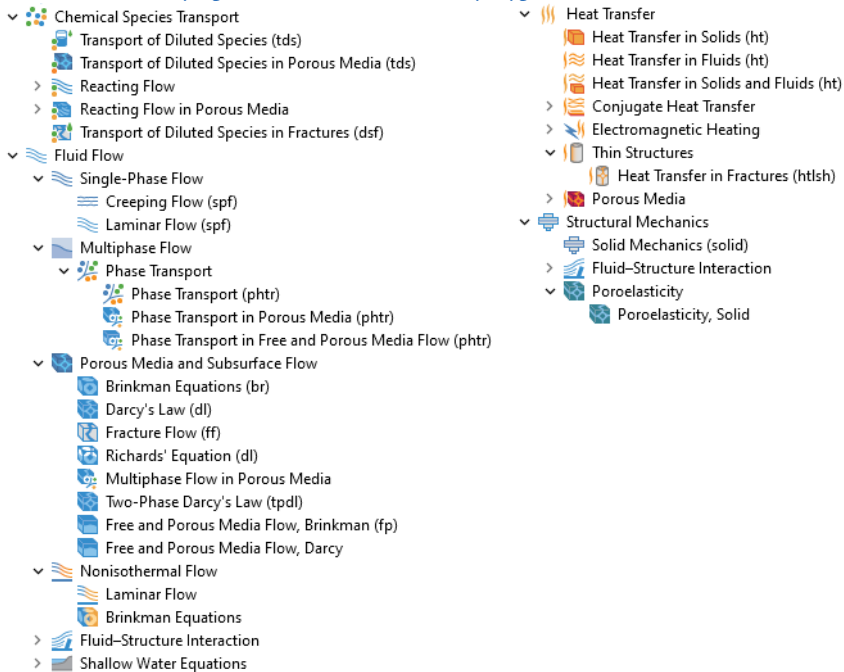 - Poroelasticity
    - Poroelasticity, Solid

Figure 1: The physics interfaces for the Subsurface Flow Module as shown in the Model Wizard for a 2D 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 interface (▣) under the Reacting Flow in Porous Media branch combines the functionality of the Brinkman Equations and Transport of Diluted Species in Porous Media interfaces. This multiphysics interface is primarily applied to model flow in porous media 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: 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 Creeping Flow interface (▦) under the Single-Phase Flow branch 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 Laminar Flow interface ($\approx$) under the Single-Phase Flow branch 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 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.

The Phase Transport in Porous Media interface ( ) under the Multiphase Flow branch 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 Phase Transport in Free and Porous Media Flow interface ( ) under the Multiphase Flow branch can be used to model transport of an arbitrary number of phases in coupled free and porous media flow. An absolute pressure must be supplied in the porous region and a velocity must be supplied in the free-flow region. Both can be obtained from one of the momentum conservation interfaces or be specified manually.

The Laminar Flow interface ($\approx$) under the Nonisothermal Flow branch is primarily applied to model flow at low to intermediate Reynolds numbers in situations where the temperature and flow fields have to be coupled. A typical example is natural convection, where thermal buoyancy forces drive the flow. This is a multiphysics interface for which the nonlocal couplings between fluid flow and heat transfer are set up automatically.

The Brinkman Equations interface ( ) under the Nonisothermal Flow branch is used to model flow in porous media in situations where the temperature and flow fields have to be coupled. This is a multiphysics interface for which the nonlocal couplings between porous media flow and heat transfer are set up automatically.

The Shallow Water Equations, Time Explicit interface ( ) under the Shallow Water Equations branch is used for modeling flow below a free surface under the condition that the horizontal length scale is much greater than the vertical length scale. The physics interface available in 2D solves the Shallow Water equations, obtained by depth averaging the Navier–Stokes equations. The dependent variables are the water depth and water flux.

POROUS MEDIA FLOW

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, Brinkman 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 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 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 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 Free and Porous Media Flow, Brinkman 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, Darcy interface ( ) provides such a coupling to model porous media flow connected to free flow domains. This multiphysics interface couples the Laminar Flow interface with the Darcy's Law interface over their common boundary.

The Free and Porous Media Flow, Brinkman and the Free and Porous Media Flow, Darcy interfaces are 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.

The Heat Transfer in Fractures interface ( ) under the Thin structures branch combines the heat conduction and convection in a thin porous system. This physics interface provides mixing rules for calculating the effective heat transfer properties of porous media.

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, Solid 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 Multiphysics basic license.

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

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Phase Transport in Porous Media		phtr	all dimensions	stationary; time dependent
Phase Transport in Free and Porous Media Flow		phtr	all dimensions	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		ff	3D, 2D, 2D axisymmetric	stationary; time dependent
Richards' Equation		dl	all dimensions	stationary; time dependent
Multiphase Flow in Porous Media		—	all dimensions	stationary; time dependent
Two-Phase Darcy's Law		tpdl	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Brinkman		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Darcy		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Flow				
Brinkman Equations		—	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF
Shallow Water Equations				
Shallow Water Equations, Time Explicit		swe	1D and 2D	time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
〽 Heat Transfer				
Heat Transfer in Solids		ht	all dimensions	stationary; time dependent
Heat Transfer in Fluids[1]		ht	all dimensions	stationary; time dependent
Heat Transfer in Solids and Fluids[1]		ht	all dimensions	stationary; time dependent
Heat Transfer in Fractures		htlsh	3D, 2D, 2D axisymmetric	stationary; time dependent; thermal perturbation, frequency domain
Heat Transfer in Porous Media		ht	all dimensions	stationary; time dependent
⬚ Structural Mechanics				
⬚ Poroelasticity				
Poroelasticity, Solid[2]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
[1] This physics interface is included with the core COMSOL Multiphysics software but has added functionality for this module.				
[2] This physics interface is a predefined multiphysics coupling that automatically adds all the physics interfaces and coupling features required.				

Tutorial Model: Pesticide Transport and Reaction in Soil

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.
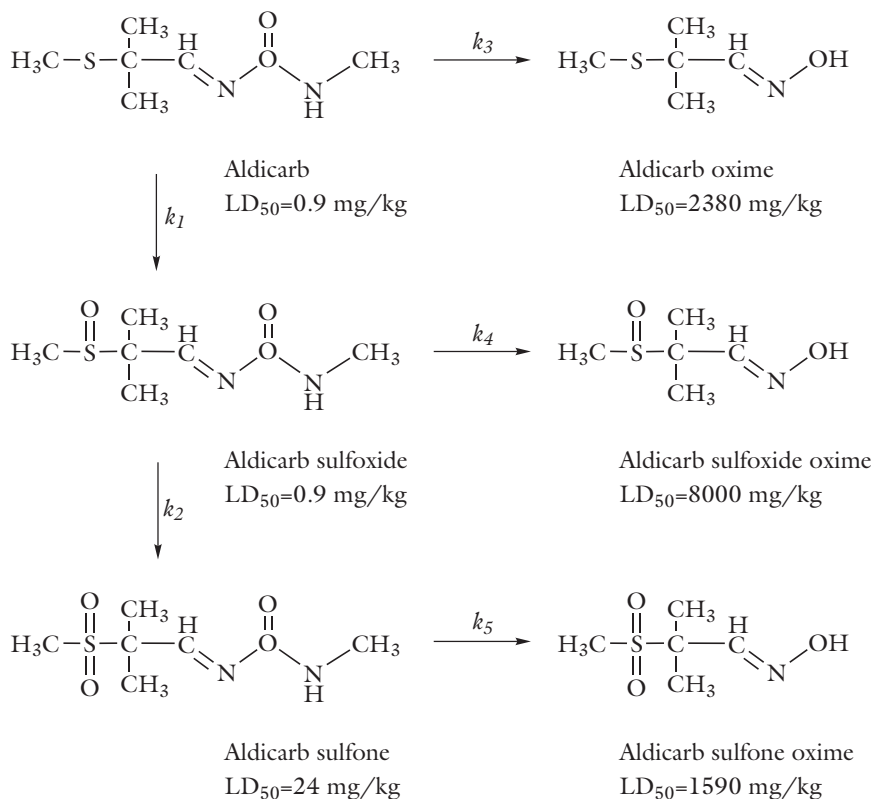
The chain of reactions is illustrated in Figure 2.

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})

$$\frac{dc_{asx}}{dt} = r_1 - r_2 - r_4 = k_1 c_a - k_2 c_{asx} - k_4 c_{asx} \qquad (3)$$

- For aldicarb sulfone (c_{asn})

$$\frac{dc_{asn}}{dt} = r_2 - r_5 = k_2 c_{asx} - k_5 c_{asn} \qquad (4)$$

- For aldicarb oxime (c_{ao})

$$\frac{dc_{ao}}{dt} = r_3 = k_3 c_{ao} \qquad (5)$$

- For aldicarb sulfoxide oxime (c_{asxo})

$$\frac{dc_{asxo}}{dt} = r_4 = k_4 c_{asx} \qquad (6)$$

- For aldicarb sulfone oxime (c_{asno})

$$\frac{dc_{asno}}{dt} = r_5 = k_5 c_{asn} \qquad (7)$$

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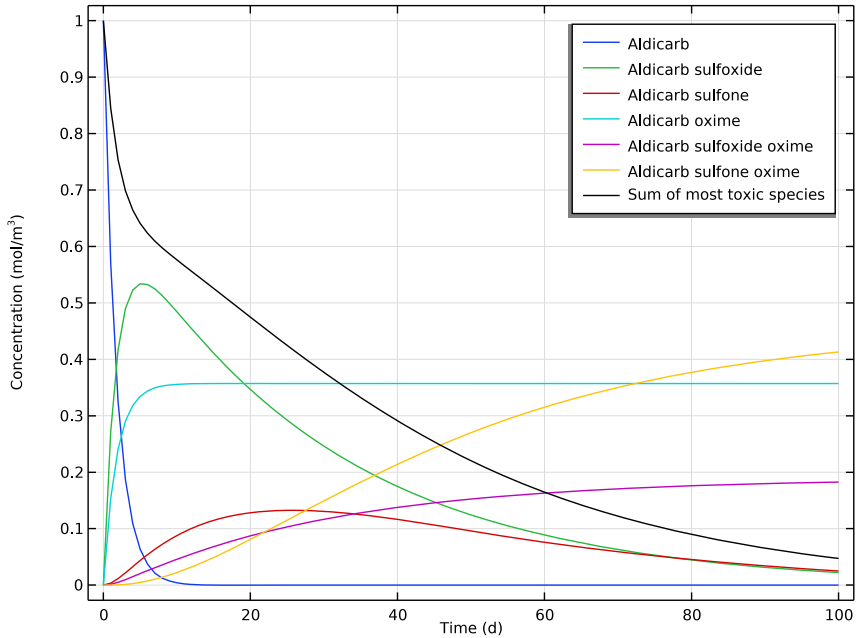
Figure 3: Concentration profiles as reactions occur during a 100 day time period. Concentration transients of the most toxic species, aldicarb (c_a), aldicarb sulfoxide (c_{asx}), aldicarb sulfone (c_{asn}), and the sum of them

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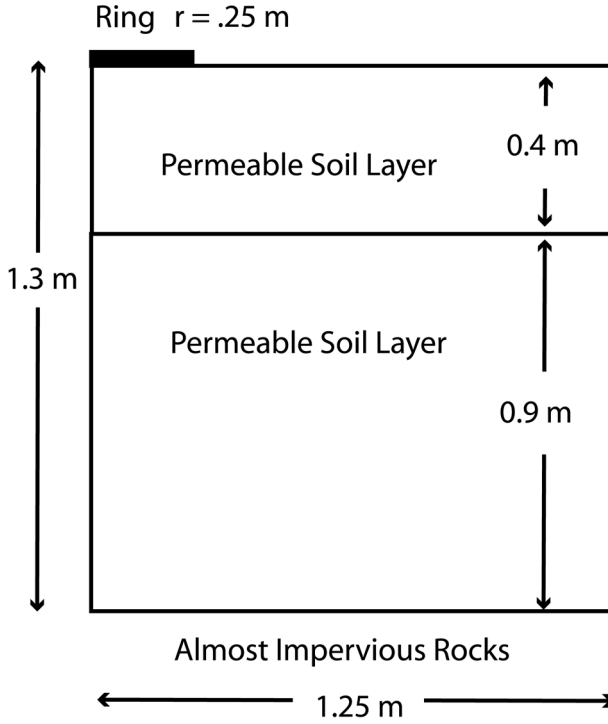
Figure 4: Geometry of the infiltration ring and soil column.

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

$$(C_m + S_e S_p)\frac{\partial H_p}{\partial t} + \nabla \cdot (-K\nabla(H_p + D)) = 0 \tag{8}$$

where C_m denotes specific moisture capacity (m^{-1}); S_e is the effective saturation of the soil (dimensionless); S_p 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); and D is the direction (typically, the z direction) that represents the vertical elevation (m).

In COMSOL Multiphysics, all equations are formulated with the pressure variable (SI unit: Pa) as dependent variable, while offering the automatic computation and accessibility of pressure head and hydraulic head for seamless integration as boundary condition or for evaluation in the results.

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 C_m and the effective saturation S_e 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

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

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

In these equations, D_{LGii} are the principal components of the water-air 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 dispersivity; D_m and D_G (m²/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_{Li}, partition coefficients, k_{Pi}, and volatilization constants, k_{Gi}. 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 effective saturation and 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.
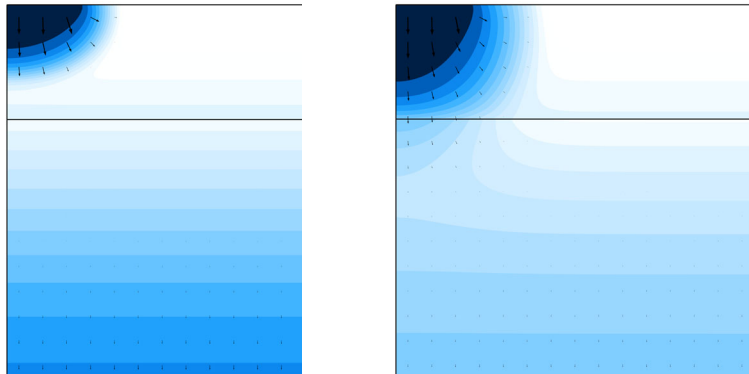
Figure 5: The effective saturation (surface plot), pressure head (contours), and flow velocity (arrows) in a variably saturated soil after 0.3 days (left) and 1 day (right).

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.
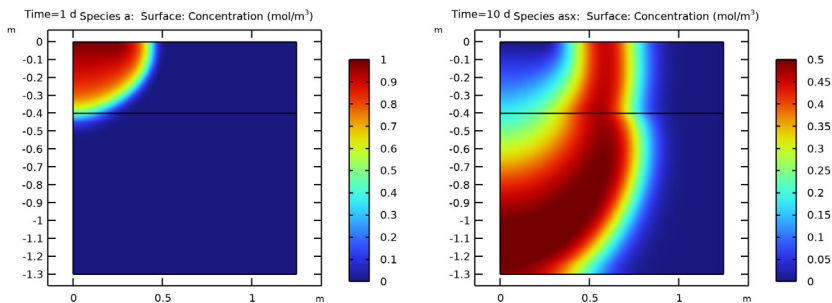
Figure 6: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 1 day.
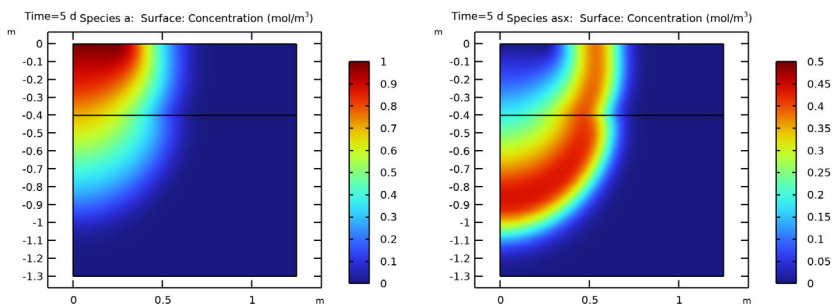
Figure 7: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 5 days.
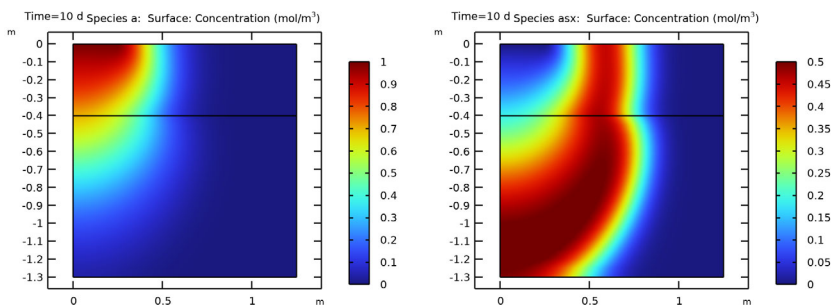
Figure 8: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 10 days.

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.

References

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 Multiphysics model or Blank Model to create one manually. For this tutorial, click the Model Wizard button.

If COMSOL Multiphysics 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) $\frac{d}{dt}$ 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\COMSOL62\Multiphysics\applications\.`

Parameters

1 In the Model Builder window, under Global Definitions click Parameters 1 P~i~ .

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.

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 (Δu).

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.

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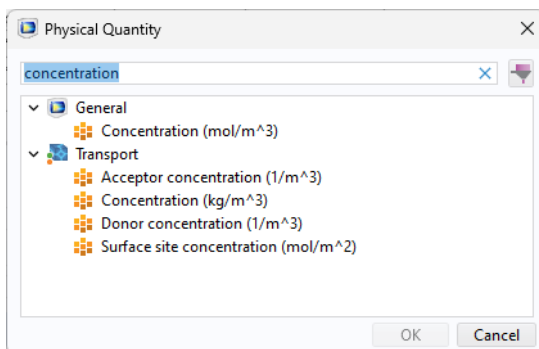
The chemical reactions (given by Equation 2 through Equation 7) are slightly modified. All the terms are moved to the left-hand side. Also note that the initial values are zero for all the concentrations, except for aldicarb.

Study 1

Time Dependent

1 In the Model Builder under the Study 1 node click Step 1: Time Dependent 📈 .

2 Go to the Settings window, under Study Settings, select d (for days) from the Time unit list.

Study Settings

Time unit:	d
Output times:	range(0,1,100) d
Tolerance:	Physics controlled

3 In the Times text field enter range(0,1,100).

4 In the Home toolbar click Compute = .

You can also right-click Study 1 ∾ in the Model Builder and select Compute = .
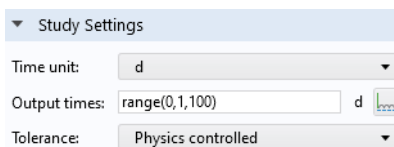
Note: On Linux and Mac, the Home toolbar refers to the specific set of controls near the top of the Desktop.

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 ∿. In the Graphics window the Global plot 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.

y-Axis Data

| 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 ⊡ to update the plot in the Graphics window and compare with Figure 3.

Now solve the space and time-dependent transport and reaction of solutes. For this purpose, the required interfaces are added. Note that the first study solved the coupled ODEs that describe the reactions. A new Study will be used for the coupled transport system.

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

6 Go to the Add Physics window. In the Physics tree, under Fluid Flow>Porous Media and Subsurface Flow, select Richards' Equations (dl). Find the Physics interfaces in study section immediately below the tree (scroll down if necessary), and clear the Solve check box for this physics interface in Study 1.

7 Click Add to Component 1.

8 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 clear the Solve check box to deactivate this physics interface in Study 1.

9 Click to expand the Dependent variables section immediately below the Physics interfaces in study section. In the Number of species text field, type 3. Change the default names to c_a, c_asx, and c_asn.
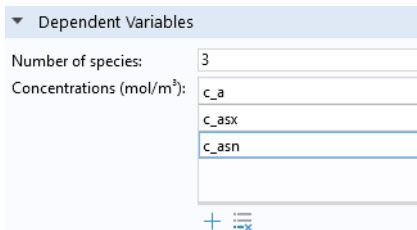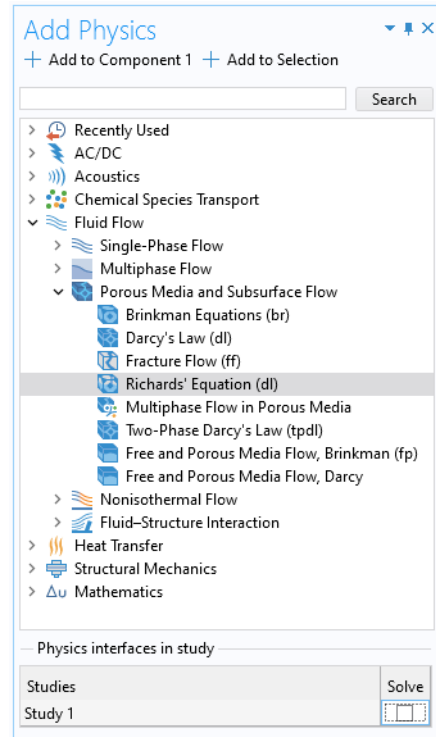
10 Click the Add to Component 1 button.

11 In the Home toolbar click Add Physics ⚛ to close the Add Physics window.

Next, add a new time-dependent study for solving the recently added interfaces.

12 In the Home toolbar click Add Study 🔗.

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

14 Go to the Physics interfaces in study section and clear the Solve check box for the Global ODEs and DAEs (ge) $\frac{d}{dt}$ interface.

15 Click the Add Study button ➕

16 In the Home toolbar click Add Study 🔗 to close the Add Study window.
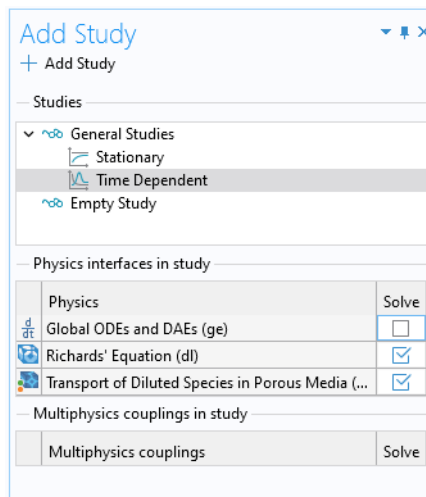
Parameters and Variables

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.

Parameters

1 In the Model Builder right-click on Global Definitions 🌐 and select Parameters P_i .

This adds a new Parameters 2 node. Alternatively, all parameters can also be stored in one single list. Using multiple parameter lists is beneficial for clarity especially if you rename the parameter lists. To do so, go the Settings window for the Parameters 2 node and type `Transport parameters` in the Label text field at the top. Rename the Parameters 1 node to `Rate constants`.

2 In the Settings window for Transport 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.

▼ Parameters

Name	Expression	Value	Description
rhof	1e3[kg/m^3]	1000 kg/m³	Fluid density
poro_1	0.339	0.339	Porosity, layer 1
poro_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
Sp_1	0.339[1/m]/(g_const*rhof)	3.4568E-5 1/Pa	Storage coefficient, layer 1
Sp_2	0.399[1/m]/(g_const*rhof)	4.0687E-5 1/Pa	Storage coefficient, layer 2
Ks_1	0.454[m/d]	5.2546E-6 m/s	Saturated hydraulic conductivity, layer 1
Ks_2	0.298[m/d]	3.4491E-6 m/s	Saturated hydraulic conductivity, layer 2
alpha_1	1.39[1/m]	1.39 1/m	Van Genuchten parameter alpha, layer 1
alpha_2	1.74[1/m]	1.74 1/m	Van Genuchten parameter alpha, layer 2
n_1	1.6	1.6	Van Genuchten parameter n, layer 1
n_2	1.38	1.38	Van Genuchten parameter n, layer 2
Hp0	0.01[m]	0.01 m	Pressure head in the ring
N0	0.01*Ks_1*rhof	5.2546E-5 kg/(m²·s)	Leak from the base
c0	1[mol/m^3]	1 mol/m³	Solute concentration in the ring
rhob	1300[kg/m^3]	1300 kg/m³	Bulk density
kp_a	1e-4[m^3/kg]	1E-4 m³/kg	Partition coefficient, aldicarb
kp_asx	0.5e-4[m^3/kg]	5E-5 m³/kg	Partition coefficient, aldicarb sulfoxide
kp_asn	2e-4[m^3/kg]	2E-4 m³/kg	Partition coefficient, aldicarb sulfone
Dl	3.74e-3[m^2/d]	4.3287E-8 m²/s	Diffusion coefficient, liquid phase
Dg	0.432[m^2/d]	5E-6 m²/s	Diffusion coefficient, gas phase
alphar	0.005[m]	0.005 m	Longitudinal dispersivity
alphaz	0.001[m]	0.001 m	Transverse dispersivity
kg_a	1.33e-7	1.33E-7	Volatilization
kg_asn	1.33e-3	0.00133	Volatilization
d_s	0.05[m]	0.05 m	Thickness of the concentration boundary layer

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. It performs a coordinate scaling to the selected domain such that boundary conditions on the

| 31

outside of the infinite element layer are effectively applied at a very large distance. Therefore unwanted effects of artificial boundary conditions on the region of interest are suppressed.

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, clear the Layers on bottom check box and type `0.25` in the Thickness text field.

These additional layers to the right of the geometry will be used to define Infinite Element Domains.

5 Under the Geometry node right-click on Rectangle 1 ▢ and choose Duplicate (⊡).

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

- In the Height text field type `0.4`.
- Under Position in the z text field, enter `-0.4`.

▼ Size and Shape		
Width:	1.5	m
Height:	0.9	m
▼ Position		
Base:	Corner	▼
r:	0	m
z:	-1.3	m
▷ Rotation Angle		
▼ Layers		

|	Layer name	Thickness (m)
	Layer 1	0.25
	Layer 2	

↑ ↓ ≡ˣ ⊡ ▼
☐ Layers to the left
☑ Layers to the right
☐ Layers on bottom
☐ Layers on top

To finish the model geometry, add a point on the top boundary to make the pond's outer rim.

7 Right-click Geometry 1 ⋏. Go to More Primitives and select Point ⋅.

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

9 Click Build All Objects 🔳 .
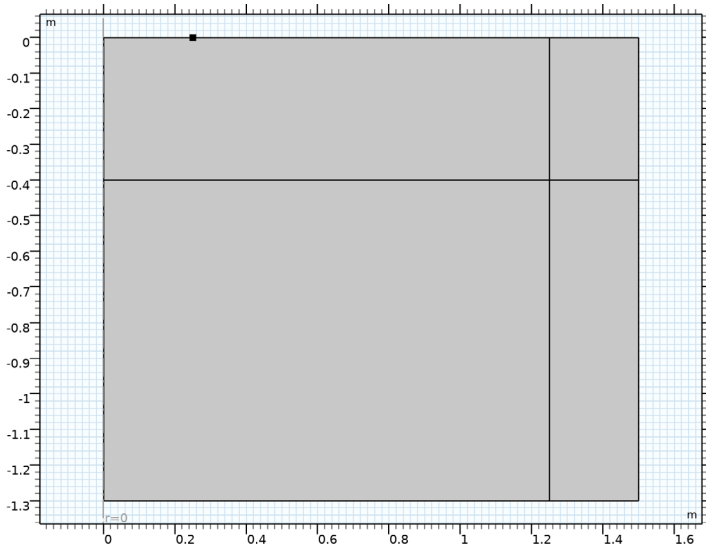
Definitions

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, locate the Geometry section and choose Cylindrical.

Variables 1

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

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,
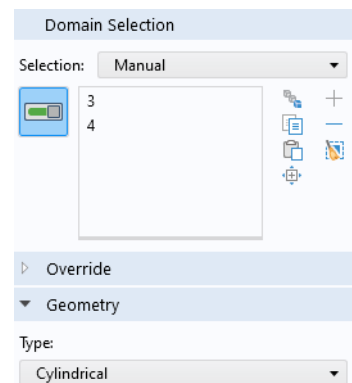
Subsurface_Flow_Module\Solute_Transport. Double-click to add or click Open.

The rate expressions are added to the table.

▼ Variables

| ⏩ Name	Expression	Unit	Description
r_1	k_1*c_a	mol/(m³·s)	Rate expression 1
r_2	k_2*c_asx	mol/(m³·s)	Rate expression 2
r_3	k_3*c_a	mol/(m³·s)	Rate expression 3
r_4	k_4*c_asx	mol/(m³·s)	Rate expression 4
r_5	k_5*c_asn	mol/(m³·s)	Rate expression 5

↑ ↓ 🔲▼ 🗐 🗐 🖊 📁▼ 💾 🔳▼

Richards' Equation

Begin by specifying the properties for the bottom soil layer in the default Unsaturated Porous Medium node, then duplicate this node and modify the domain selection and properties to match the top layer.

Unsaturated Porous Medium I

1 In the Model Builder under the Richards' Equation interface 🔯 , click the Unsaturated Porous Medium 1 node.

˅ 🔯 Richards' Equation (dl)
  ˅ 🔲 Unsaturated Porous Medium 1
    🔲 Fluid 1
    🔲 Porous Matrix 1

2 Locate the Porous Medium Section and from the Storage model list select User Defined.

3 In the S_p text field, type Sp_1.

The Fluid subnode under the Unsaturated Porous Medium node uses default values for the material properties. The material properties will be defined later.

▼ Porous Medium

Storage model:

User defined	▼

S_p | Sp_1 | 1/Pa
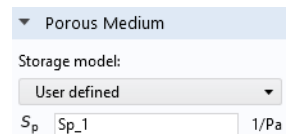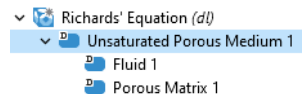
4 Go to the Porous Matrix subnode and locate the Matrix Properties section:

- From the Permeability model list, select Hydraulic conductivity. In the K_s text field, enter `Ks_1`.

5 Under Retention Model:

- Keep 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.

- Enter `thetar_1` in the θ_r text field for the residual liquid volume fraction.

Matrix Properties

Porosity:

ϵ_p From material ▼

Permeability model:

   Hydraulic conductivity ▼

K_s Ks_1   m/s

   Isotropic ▼

Retention Model

Retention model:

   van Genuchten ▼

α alpha_1   1/m

n n_1   1

l 0.5   1

Residual liquid volume fraction:

θ_r thetar_1   1

Unsaturated Porous Medium 2

1 In the Model Builder right-click Unsaturated Porous Medium 1. Select Duplicate ⊞.

2 In the Settings window verify that the Domain Selection consists of domains 2 and 4 only (the upper layer). Select 1 and 3 in the list and click on the Remove from Selection — button.

3 Locate the Porous Medium section. In the S_p text field, type `Sp_2`.

4 Select the Porous Matrix subnode and locate the Matrix Properties section:

- In the K_s text field, enter `Ks_2`.

5 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.

- Enter `thetar_2` in the θ_r text field for the residual liquid volume fraction.

Gravity 1

For the Richards' Equation interface Gravity is active by default.

1 Go to the Gravity 1 node under Richards' Equation (dl).

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

> **Gravity**
>
> Specify:
>
> | Elevation | ▼ |
>
> Elevation:
>
> D | z | m
>
> Acceleration of gravity:
>
> g | g_const | m/s²
>
> ☐ Specify reference position

Initial Values 1

1 Select the Initial Values 1 node 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 Right-click the Initial Values 1 node and choose Duplicate ⊞.

2 In the Settings window for Initial Values 2 under Domain Selection, select Domains 2 and 4 (upper layer) only.

3 Locate the Initial Values section. In the H_p text field, enter the expression -(z+1.2)-0.2*(z+0.4).

> ✓ 🔲 Richards' Equation (dl)
> > 🔳 Unsaturated Porous Medium 1
> > 🔳 Axial Symmetry 1
> > 🔳 No Flow 1
> > 🔳 Gravity 1
> > 🔳 Initial Values 1
> > 🔳 Unsaturated Porous Medium 2
>
> ▼ Initial Values
>
> ○ Pressure
>
> p | 0
>
> ● Pressure head
>
> H_p | -(z+1.2)
>
> ○ Hydraulic head
>
> H | 0

Next, define the boundary conditions for the Richards' Equation interface.

Pressure Head 1

1 In the Model Builder click Richards' Equation (dl) 🔲. In the Physics toolbar click Boundaries ⬭ and select Pressure Head. Alternatively, right-click on Richards' Equation (dl) 🔲 and select Pressure Head from the menu.

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

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

> ▼ Pressure Head
>
> Pressure head:
>
> H_{p0} | Hp0 | m

Pervious Layer 1

4 In the Physics toolbar click Boundaries ⬭ and select Pervious Layer.

5 In the Boundary Selection window, select Boundaries 2 and 8 only. These are the boundaries at the bottom.

6 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.

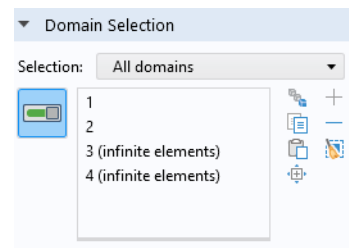This concludes the setup of the Richards' Equation interface.
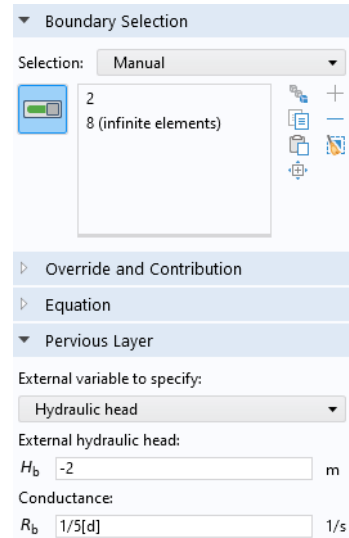
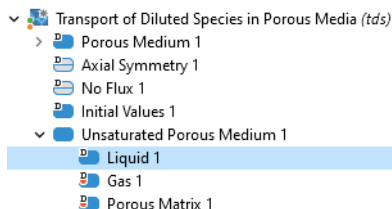## Transport of Diluted Species in Porous Media

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.

Unsaturated Porous Medium 1

1 In the Model Builder under Component 1, click Transport of Diluted Species in Porous Media (tds) 🔷 .

2 In the Physics toolbar click Domains ⬤ and select Unsaturated Porous Medium.

3 In the Settings window for Unsaturated Porous Medium, under Domain Selection select All domains from the Selection list.

4 Select Liquid under the Unsaturated Porous Medium node.

Transport of Diluted Species in Porous Media (tds)
> Porous Medium 1
Axial Symmetry 1
No Flux 1
Initial Values 1
Unsaturated Porous Medium 1
Liquid 1
Gas 1
Porous Matrix 1

5 In the Settings window for Liquid, under Saturation change from Saturation to Liquid volume fraction, then enter `dl.theta_l` in the θ_l text field. This is the name for the liquid volume fraction calculated with the Richards' Equation interface

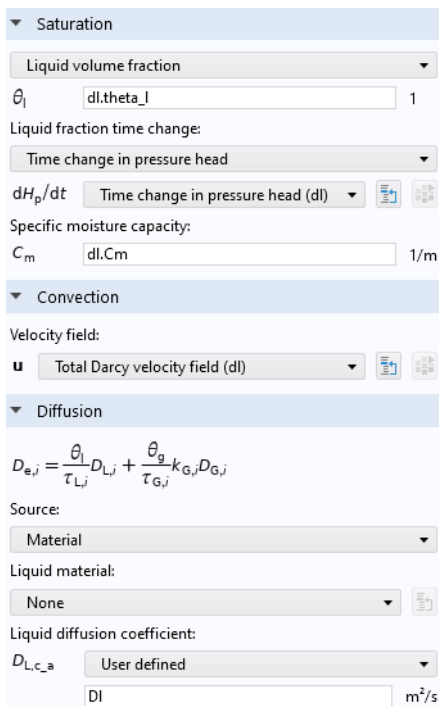**6** From the Liquid fraction time change list, choose
Time change in pressure head. In the dH_p/dt list, select
Time change in pressure head (dl).

This is the variable from the Richards' Equation interface.

7 Under Specify moisture capacity, enter `dl.Cm` in the C_m text field.

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

9 The diffusion coefficients are identical for all species. Enter `Dl` in the text fields for D_{L,c_a}, D_{L,c_asx}, and D_{L,c_asn}.

▼ Saturation

Liquid volume fraction

θ_l dl.theta_l   1

Liquid fraction time change:

Time change in pressure head

dH_p/dt Time change in pressure head (dl)

Specific moisture capacity:

C_m dl.Cm   1/m

▼ Convection

Velocity field:

u   Total Darcy velocity field (dl)

▼ Diffusion

$$D_{e,i} = \frac{\theta_l}{\tau_{L,i}} D_{L,i} + \frac{\theta_g}{\tau_{G,i}} k_{G,i} D_{G,i}$$

Source:

Material

Liquid material:

None

Liquid diffusion coefficient:

D_{L,c_a} User defined

DI   m²/s

10 Select the Gas 1 subnode under Unsaturated Porous Medium 1.

11 The gas diffusion coefficients are identical for all species. Enter `Dg` in the text fields for D_{Gc_a}, D_{G,c_asx}, and D_{G,c_asn}.

12 Find the Volatilization section and enter `kg_a` in the text field for k_{G,c_a} and `kg_asn` in the text field for k_{G,c_asn}.

The Porous Matrix 1 subnode keeps the default settings.

▼ Volatilization

k_{G,c_a}	kg_a	1
k_{G,c_asx}	0	1
k_{G,c_asn}	kg_asn	1

Adsorption 1

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

2 In the Settings window for Adsorption, locate the Adsorption section and select User defined from the Adsorption isotherm list.

3 Select the check box for c_a. In the $c_{P,ca}$ text field, enter `kp_a*c_a`.

4 Select the check box for c_asx. In the $c_{P,casx}$ text field, enter `kp_as*c_asx`.

▼ Adsorption

$c_{P,i} = f(c_i)$

Adsorption isotherm:

User defined	▼

☑ Species c_a

c_{P,c_a}	kp_a*c_a	mol/kg

☑ Species c_asx

c_{P,c_asx}	kp_asx*c_asx	mol/kg

☑ Species c_asn

c_{P,c_asn}	kp_asn*c_asn	mol/kg

5 Select the check box for c_asn. In the $c_{P,casn}$ text field, enter `kp_asn*c_asn`.

Dispersion

1 Right-click Unsaturated Porous Medium 1 and choose Dispersion.

2 For the Dispersion tensor list, select Dispersivity. For the Dispersivity model list, select Transverse isotropic. Enter `alphar` and `alphaz`.

Reactions 1

1 In the Physics toolbar click Domains ⬤ and select Reactions.

▼ Dispersion

☐ Specify dispersion for each species individually

Dispersion tensor:

Dispersivity	▼

$D_{D,i} = D_{D,i}(\alpha)$

Dispersivity model:

Transverse isotropic	▼

Dispersivity:

α	alphar	m
	alphaz	

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_l*(-r_1-r_3)`.

- In the R_{c_asx} text field, enter
  `dl.theta_l*(r_1-r_2-r_4)`.

- In the R_{c_asn} text field, enter
  `dl.theta_l*(r_2-r_5)`.

Outflow 1

1 In the Physics toolbar click Boundaries ⊖ and select Outflow.

2 In the Settings window for Outflow locate the Boundary Selection section and select boundaries 2, 8, 12, and 13 only. This corresponds to the bottom and right boundaries.

Concentration 1

1 In the Physics toolbar click Boundaries ⊖ and select Concentration.

2 In the Settings window for Concentration locate the Boundary Selection section. Select 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`.

Volatilization 1

1 In the Physics toolbar click Boundaries ⊖ and select Volatilization.

2 In the Settings window locate the Boundary Selection section. Select boundaries 6 and 11 only.

3 In the Volatilization section, enter `Dg/d_s` in the h_c text field.

4 Select the Species c_a check box.

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

5 Select the Species c_asn check box.

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

Materials

Not all material properties have been defined in the physics features. It is convenient to define the material properties in a porous material. Since both interfaces can access these materials, duplicate definitions, such as porosity, are avoided.

Porous Material: Lower Layer

1 In the Model Builder window, under Component 1 (comp1) right-click Materials ⊞ and choose More Materials>Porous Material ⊞.

2 In the Settings window for Porous Material, type
`Porous Material: Lower Layer` in the Label text field.

Renaming nodes is optional. It is mainly for clarity and helps to quickly understand the model.

3 Locate the Phase-Specific Properties section. Click the Add Required Phase Nodes ⊞ button.

This adds the required subnodes to define the fluid properties and solid matrix properties.

✓ ⊞ Materials
  ✓ ⊞ Porous Material: Lower Layer *(pmat1)*
    > ⊞ Fluid 1 *(pmat1.fluid1)*
    > ⊞ Solid 1 *(pmat1.solid1)*
    ⊞ Basic *(def)*

4 Go to the Fluid 1 ⊞ subnode. Locate the Material contents section and in the table enter `rhof` for the Density.

	Property	Variable	Value	Unit	Property group
☑	Density	rho	rhof	kg/m³	Basic
	Porosity	epsilon	0.339	1	Porous model

5 Click on the Solid 1 ⊞ subnode and locate the Solid Properties section. Enter `1-poro_1` in the Volume fraction text field.

6 In the Material Contents section, in the table enter `rhob` for the Density.

	Property	Variable	Value	Unit	Property group
☑	Density	rho	rhob	kg/m³	Basic
	Porosity	epsilon	0.339	1	Porous model

Porous Material: Upper Layer

1 In the Model Builder right-click Porous Material: Lower Layer and select Duplicate ⊕.

2 In the Settings window for Porous Material, type `Porous Material: Upper Layer` in the Label text field.

3 In the Settings window, under Domain Selection, select Domains 2 and 4 (upper layer) only.

4 Expand the Porous Material: Upper Layer node, then click Solid 1 ⊟.

5 In the Settings window, locate the Solid Properties section. In the θ_s text field, type `1-poro_2`.

All other material properties remain identical to the ones defined for the lower layer. This completes the setup of the physics.

Mesh

Using a Mapped mesh is a good idea for this geometry. It uses less mesh elements while keeping the accuracy compared to using a triangular mesh with the same mesh size.

1 In the Model Builder click Mesh 1 ◭. In the Settings window, locate the Physics-Controlled Mesh section. From the Element Size list, choose Finer.

2 In the Mesh toolbar, click Mapped ▦.

3 Right-click Mapped 1 ⬚ and select Size ◭.

4 In the Settings window for Size, locate the Geometric Entity Selection section. From the Geometric entity level list, select Domain and choose Domain 2 only.
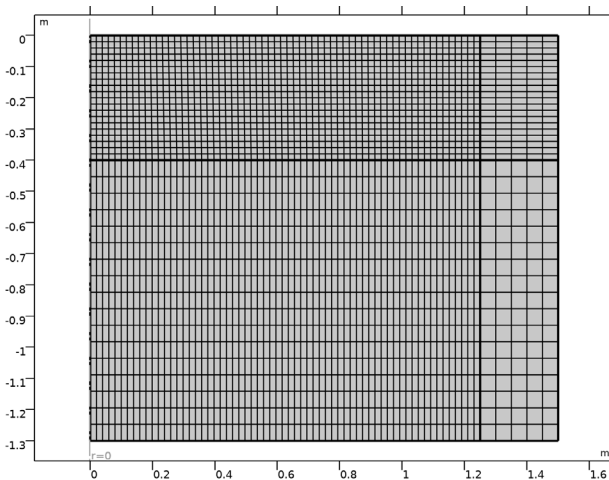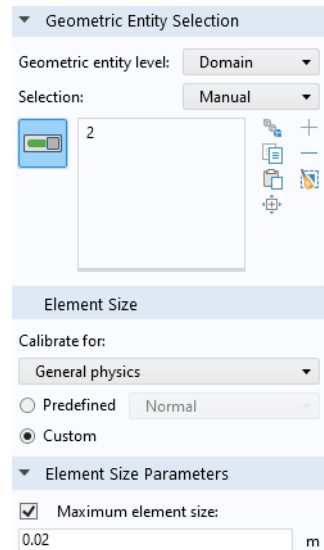
In Domain 2, the meshing should be finer to accurately resolve the transport of pesticides. All other domains will be meshed with the setting from the top Size node.

5 In the Element Size section click the Custom button.

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

7 In the associated text field, type `0.02`.
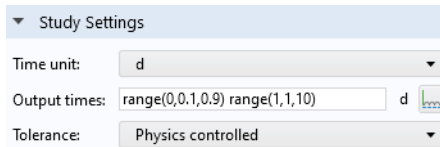
8 Click Build All ⬚ .

▾	Geometric Entity Selection
Geometric entity level:	Domain
Selection:	Manual

2

Element Size
Calibrate for:
General physics
◯ Predefined   Normal
⦿ Custom

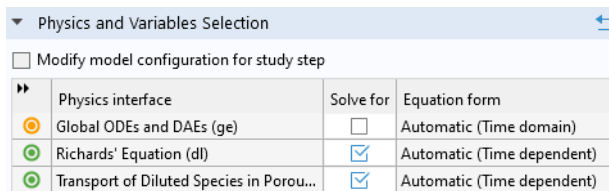| ▾	Element Size Parameters
☑	Maximum element size:

| 0.02 | m |

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 (days) 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).

Study Settings		
Time unit:	d	
Output times:	range(0,0.1,0.9) range(1,1,10)	d
Tolerance:	Physics controlled	

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 Study 2. The ODEs are already solved in Study 1.

▼ Physics and Variables Selection			↩
☐ Modify model configuration for study step			
⤸ Physics interface	Solve for	Equation form	
⦿ Global ODEs and DAEs (ge)	☐	Automatic (Time domain)	
⦿ Richards' Equation (dl)	☑	Automatic (Time dependent)	
⦿ Transport of Diluted Species in Porou...	☑	Automatic (Time dependent)	

5 In 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 under Results 🖥 expand the Data Sets ⠿ node.

2 Right-click Study2/Solution 2 ⠿ , and select Selection 🐾 .

3 In the Settings window locate the Geometric Entity Selection section. From the Geometric entity level list, choose Domain.

4 Select Domain 1 and 2 only. This will remove the Infinite Element domains from the plot groups.

> ∨ 🖥 Results
>   ∨ ⠿ Datasets
>   ⠿ Study 1/Solution 1 *(sol1)*
>   ∨ ⠿ Study 2/Solution 2 *(sol2)*
>   🐾 Selection
>   🖫 Revolution 2D
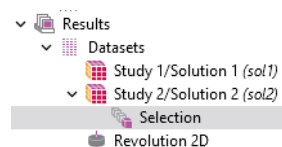
Add a new plot to show the effective saturation, pressure head, and velocity field at different times. For the effective saturation a predefined plot is available.

Effective saturation

1 In the Results toolbar click Add Predefined Plot ▣ .

2 Go to the Add Predefined Plot window and expand the Richard's Equation node under Study 2/Solution 2. Double-click on Effective Saturation.

This adds the plot to the Results node.

3 Go to the Settings window and locate the Data section. From the Time(d) list choose 0.3.
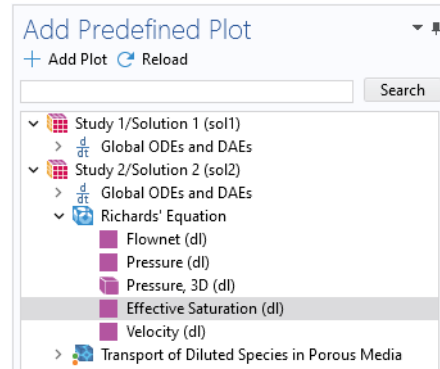
4 Expand the Effective Saturation node and go the Contour node.

5 In the Settings window, locate the Levels section and type 15 in the Total Levels text field.

6 Click the Effective saturation node. On the Effective saturation toolbar click Arrow Surface ▣ .

7 In the Settings window, verify that `dl.u` and `dl.w` are the expressions in the R- and Z- component text fields.

These are the components of Darcy's velocity field.

8 Locate the Coloring and Style section and from the Color list, choose Black.

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

10 Click Effective saturation. In the Settings window, locate the Data section and from the Time list choose 1 day.

11 Click Plot ▣ . Compare the plot in the Graphics window with that in the right panel of Figure 5.
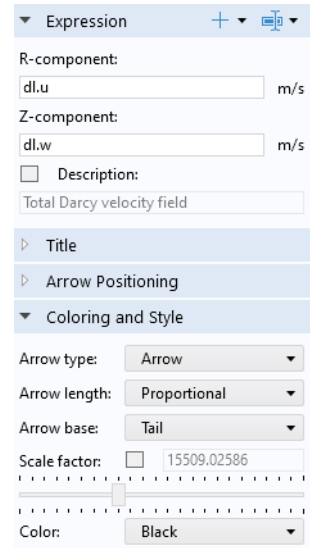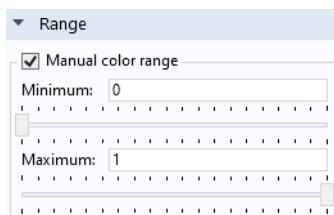
Concentration, aldicarb

1 In the Model Builder under Results click on the Concentration, a (tds) node. In the Settings window, type `Concentration, aldicarb` in the Label text field.

2 Expand the Concentration, aldicarb node.

3 Right-click on the Streamline 1 (≋)node and choose Disable ⊘ .

4 Click on the Surface 1 ■ node. In the Settings window for 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.

> ▼ Range
>
> ☑ Manual color range
>
> Minimum: 0
>
> Maximum: 1

This gives a single color range for all the concentration plots.

5 Click the Plot 🔲 button.

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.

6 In the Model Builder under Results click Concentration, aldicarb.

7 In the Settings window locate the Data section, and from the Time list choose 5 days. Click Plot 🔲 .

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

Concentration, aldicarb sulfoxide

1 In the Model Builder under Results click on Concentration, asx (tds), and in the Settings window, type `Concentration, aldicarb sulfoxide` in the Label text field.

2 Expand the Concentration, aldicarb sulfoxide node. Right-click the Streamline 1 (≋)node and choose Disable ⊘ .

3 Click on the Surface 1 ■ node. In the Settings window 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.

4 Click Plot 🔲 .

5 To reproduce the plots shown in Figure 6 through Figure 8, you can use the Plot previous ← button at the top of the Settings window to step through all available times.

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 clicking on the Animation button ▦ in the Results toolbar and select Player ▦ .