Created in COMSOL Multiphysics 6.0

Variably Saturated Flow and Transport — Sorbing Solute

Introduction

In this example, water ponded in a ring on the ground moves into a relatively dry soil column and carries a chemical with it. As it moves through the variably saturated soil column, the chemical attaches to soil particles, slowing the solute transport relative to the water. Additionally the chemical concentrations decay from biodegradation in both the liquid and the solid phase. The inspiration for the problem comes from Ref. 1.

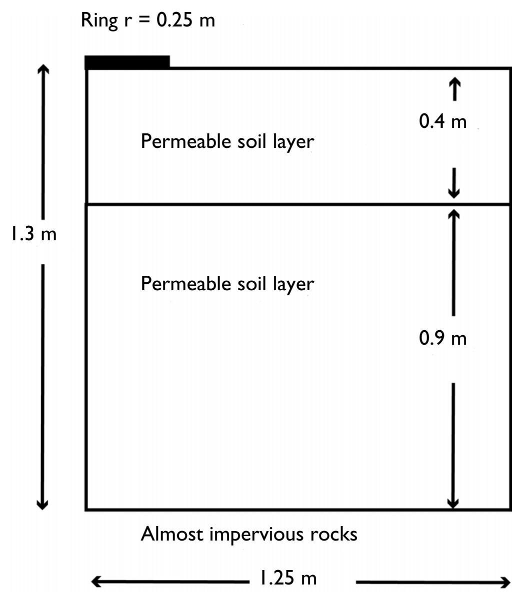


Figure 1: Geometry of the infiltration ring and soil column.

The example uses the Richards' Equation interface to define nonlinear relationships with retention and permeability properties according to van Genuchten (Ref. 2). In the Richards' Equation interface you can also define these material properties with Brooks and Corey's analytic permeability and retention formulas (Ref. 3) or by interpolation from experimental data.

Richards' equation accounts for changes in the fluid volume fraction with time, and also for changes in the storage related to variations in the pressure head according to Bear (Ref. 4). With the storage terms, the transport of diluted species in porous media equations in the Subsurface Flow Module also account explicitly for the time changes in liquid and air content.

Model Definition

The water moves from a ring on the ground into the subsurface. The 0.25-m radius ring ponds the water to a depth of 0.01 m but is open to the ground surface. Permeable soils exist to a depth of 1.3 m. The soil in the uppermost layer is slightly less permeable than the bottom one. The lower layer sits above relatively impermeable soil, so only a very small amount of leakage exits from the base. The flow is symmetric about the line $r = 0$. The initial distribution of pressure heads is known.

The water in the ring contains a dissolved solute at a constant concentration, c_0. The solute enters the ground with the water and moves through the subsurface by advection and dispersion. Additionally, the solute adsorbs or attaches to solid surfaces, which reduces the aqueous concentrations and also slows solute movement relative to the water. Microbial degradation also reduces both the liquid-phase and solid-phase concentrations. The sorption and the biodegradation are linearly proportional to aqueous concentrations. The fluid in the ring is the only chemical source, and the solute is free to leave the soil column with the fluid flux. Initially the soil is free of the solute. You track its transport for five days.

FLUID FLOW

Richards' equation governs the saturated-unsaturated flow of water in the soil. The soil air is open to the atmosphere, so you can assume that pressure changes in air do not affect the flow and use Richards' equation here for single-phase flow. Given by Ref. 4, Richards' equation in pressure head reads

$$(C_{\mathrm{m}} + S_{\mathrm{e}}S_{\mathrm{p}})\frac{\partial H_p}{\partial t} + \nabla \cdot (-K\nabla(H_p + D)) = 0$$

where C_{m} denotes specific moisture capacity (m^{-1}); $\mathrm{S_e}$ 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); D is the direction (typically, the z direction) that represents vertical elevation (m).

To be able to combine boundary conditions and sources with the Darcy's Law formulation, COMSOL Multiphysics converts Richards' equation to SI units and solves for the pressure (SI unit: Pa). Hydraulic head, H, pressure head, H_p, and elevation D are related to pressure p as

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

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

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

In this problem, $S_p = (\theta_s - \theta_r)/(1\ \mathrm{m}\cdot\rho g)$ where θ_s and θ_r denote the volume fraction of fluid at saturation and after drainage, respectively. For more details see *The Richards' Equation Interface* in the *Subsurface Flow Module User's Guide*.

With variably saturated flow, fluid moves through but may or may not completely fill the pores in the soil, and θ denotes the volume fraction of fluid within the soil. The coefficients C_m, S_e, and K vary with the pressure head, H_p, and with θ, making Richards' equation nonlinear. The specific moisture capacity, C_m, relates variations in soil moisture to pressure head as $C_m = \partial\theta/\partial H_p$. In the governing equation, C_m defines storage changes produced by varying fluid content because $C_m \partial H_p/\partial t = \partial\theta/\partial t$. Because C_m goes to zero at saturation, time change in storage relates to compression of the aquifer and water under saturated conditions. The saturated storage comes about with the effective saturation, as represented by the second term in the time-coefficient. Furthermore, K is a function that defines how readily the porous media transmits fluid. The relative permeability of the soil, κ_r, increases with fluid content giving $K = K_s\kappa_r$, where K_s (m/d) is the constant hydraulic conductivity at saturation.

This example uses predefined interfaces for van Genuchten formulas (Ref. 2) to represent how the four retention and permeability properties — θ, C_m, S_e, and $\kappa_r = K/K_s$ — vary with the solution H_p. For more details about these relationships see the section *Retention and Permeability Relationships* in the *Theory for the Richards' Equation Interface* chapter in the *Subsurface Flow Module User's Guide*.

Boundary Conditions and Initial Conditions

The problem statement records all the boundary conditions you need for this model. The level of water in the ring is known at 0.01 m, giving a Dirichlet constraint on pressure head. Approximate the small leak from the base, N_0, as $0.01K_s$. Infinite Elements are used that apply a coordinate scaling in r-direction. The boundary condition applied to these infinite elements is effectively applied at a very large distance. Together with no flow crossing the surface outside of the pressure ring or the infinite elements, the following expressions summarize the boundary conditions:

$$
\begin{array}{lll}
H_p = H_{p0} & \partial\Omega & \text{Ring} \\
\mathbf{n} \cdot \mathbf{u} = 0 & \partial\Omega & \text{Surface} \\
\mathbf{n} \cdot \mathbf{u} = 0 & \partial\Omega & \text{Sides} \\
\mathbf{n} \cdot \mathbf{u} = 0 & \partial\Omega & \text{Symmetry} \\
\mathbf{n} \cdot \rho\mathbf{u} = N_0 & \partial\Omega & \text{Base}
\end{array}
$$

In these expressions, $\mathbf{n}$ is the unit vector normal to the bounding surface, and $\mathbf{u}$ is Darcy's velocity field. The initial conditions specify the pressure head in the modeling domain as

$$
H_p = \begin{cases} -(z + 1.2\text{ m}) - 0.2(z + 0.4\text{ m}) & \text{Upper layer} \\ -(z + 1.2\text{ m}) & \text{Lower layer} \end{cases}
$$

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA

Groundwater flow and solute transport are linked by fluid velocities. With the form of the transport equation that follows, the fluid velocities need to come from Darcy's law:

$$
\mathbf{u} = K_s \kappa_r \nabla(H_p + D)
$$

In this expression, $\mathbf{u}$ is Darcy's velocity field (SI unit: m/s).

The equation that governs advection, dispersion, sorption, and decay of solutes in groundwater is

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

It describes time rate of change in two terms: c denotes dissolved concentration (mol/m^3), and c_P is the mass of adsorbed contaminant per dry unit weight of solid (mg/kg). Further, θ denotes the volume fluid fraction (porosity), and ρ_b is the bulk density (kg/m^3). Because ρ_b amounts to the dried solid mass per bulk volume of the solids and pores together, the term $\rho_b c_P$ gives solute mass attached to the soil as a concentration. In the equation, D_L is the hydrodynamic dispersion tensor (m^2/d); R_L represents reactions in water (mol/(m^3·d)); and R_P equals reactions involving solutes attached to soil particles (mol/(m^3·d)). Finally, S_c is solute added per unit volume of soil per unit time (mol/(m^3·d)).

It is far more convenient to solve the above equation only for dissolved concentration. This requires expanding the left-hand side to

$$\frac{\partial}{\partial t}(\theta c)+\frac{\partial}{\partial t}(\rho_b c_P) = \theta\frac{\partial c}{\partial t}+c\frac{\partial\theta}{\partial t}+\rho_b\frac{\partial c_P}{\partial c}\frac{\partial c}{\partial t}$$

and inserting a few definitions.

In this problem, solute mass per solid mass, c_P, relates to dissolved concentration, c, through a linear isotherm or partition coefficient k_P (m^3/kg) where $c_P = k_P c$. Because the relationship is linear, the derivative is $k_P = \partial c_P/\partial c$. Making those substitutions gives the form of the solute transport problem you solve:

$$(\theta+\rho_b k_P)\frac{\partial c}{\partial t}+c\frac{\partial\theta}{\partial t}+\mathbf{u}\cdot\nabla c+\nabla\cdot(-\theta D_L\nabla c) = \theta\phi_L c+\rho_b k_P\phi_P c+S_c$$

In the equation, ϕ_L and ϕ_P denote the decay rates (d^{-1}) for the dissolved and adsorbed solute concentrations, respectively.

Select the **Time change in pressure head** option for **Fluid fraction time change** in the **Saturation** settings for the Unsaturated Porous Media feature to employ results from the flow equation in the solute-transport model:

$$c\frac{\partial\theta}{\partial t} = cC_m\frac{\partial H_p}{\partial t}$$

Note that COMSOL Multiphysics solves for pressure, p, and converts to H_p based on the fluid weight.

The hydrodynamic dispersion tensor, D_L, describes mechanical spreading from groundwater movement in addition to chemical diffusion:

$$\theta D_{Lii} = \alpha_1\frac{u_i^2}{|\mathbf{u}|}+\alpha_2\frac{u_j^2}{|\mathbf{u}|}+\theta\frac{D_m}{\tau_L}$$

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

where D_{Lii} are the diagonal entries in the dispersion tensor; D_{Lij} are the cross terms; α is the dispersivity (m); the subscripts “1” and “2” denote longitudinal and transverse dispersivities, respectively; D_m denotes the coefficient of molecular diffusion (m^2/d); and τ_L is a tortuosity factor that reduces impacts of molecular diffusion for porous media relative to free water. Here $\tau_L = \theta^{-7/3}\theta_s^2$.

Boundary Conditions and Initial Conditions

The boundary and initial conditions in the sorbing-solute problem are straightforward. The solute enters only with the water from the ring at a concentration c_0. The solute is free to leave, but there is only minimal leakage from the lower boundary and no flow from the sides. Transport is symmetric about the line $r = 0$. The boundary conditions in this problem are:

$$
\begin{array}{ll}
c = c_0 & \partial\Omega \ \text{Ring} \\
\mathbf{n} \cdot (-\theta D_\mathrm{L} \nabla c) = 0 & \partial\Omega \ \text{Surface} \\
\mathbf{n} \cdot (-\theta D_\mathrm{L} \nabla c) = 0 & \partial\Omega \ \text{Sides} \\
\mathbf{n} \cdot (-\theta D_\mathrm{L} \nabla c + \mathbf{u} c) = 0 & \partial\Omega \ \text{Symmetry} \\
\mathbf{n} \cdot (-\theta D_\mathrm{L} \nabla c) = 0 & \partial\Omega \ \text{Base}
\end{array}
$$

where $\mathbf{n}$ is the unit vector normal to the boundary. Because the soil is pristine at the start of the experiment, the initial condition is one of zero concentration.

MODEL DATA

The following table provides data for the fluid-flow model:

VARIABLE	UNIT	DESCRIPTION	UPPER LAYER	LOWER LAYER
K_s	m/d	Saturated hydraulic conductivity	0.298	0.454
θ_s		Porosity/void fraction	0.399	0.339
θ_r		Residual saturation	0.001	0.001
α	m^{-1}	alpha parameter	1.74	1.39
n		n parameter	1.38	1.60
m		m parameter	1-1/n	1-1/n
l		Pore connectivity parameter	n/a	
H_{p0}	m	Pressure head in ring	0.01	
$H_{p,\mathrm{init}}$	m	Initial pressure head	-(z+1.2) -0.2(z+0.4)	-(z+1.2)

The inputs needed for the solute-transport model are:

VARIABLE	UNITS	DESCRIPTION	VALUE
ρ_b	kg/m^3	Bulk density	1400
k_p	m^3/kg	Partition coefficient	0.0001
D_m	m^2/d	Coefficient of molecular diffusion	0.00374
α_r	m	Longitudinal dispersivity	0.005
α_z	m	Transverse dispersivity	0.001
ϕ_L	d^{-1}	Decay rate in liquid	0.05

VARIABLE	UNITS	DESCRIPTION	VALUE
ϕ_P	d^{-1}	Decay rate on solid	0.01
c_0	mol/m^3	Solute concentration in ring	1.0

Results and Discussion

Figure 2 and Figure 3 give the solution to the fluid-flow problem at 0.3 days and 1 day, respectively. The images show effective saturation (surface plot), pressure head (contours), and velocities (arrows). The figures illustrate the soil wetting with time. As the arrows indicate, the velocities just below the ring are high relative to the remainder of the soil column.

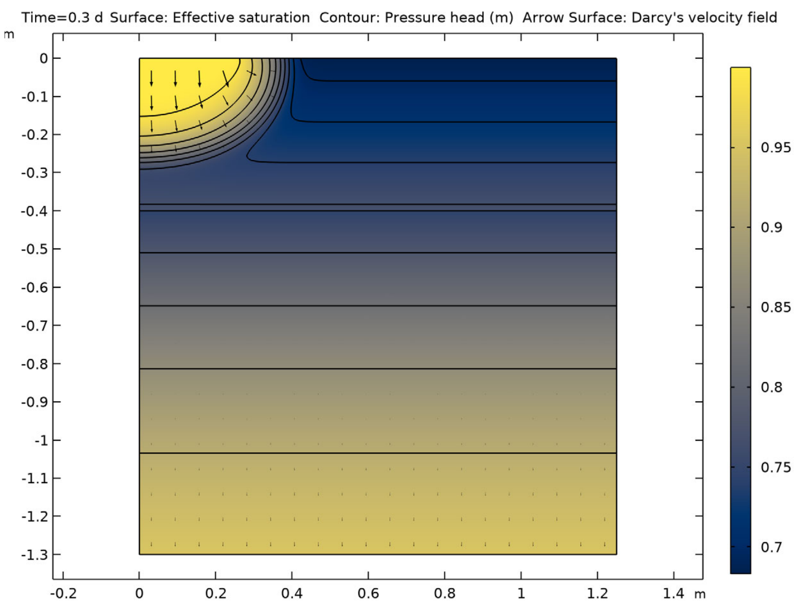


Figure 2: Estimates of effective saturation (surface plot), pressure head (contours), and velocity (arrows) in variably saturated soil after 0.3 days.

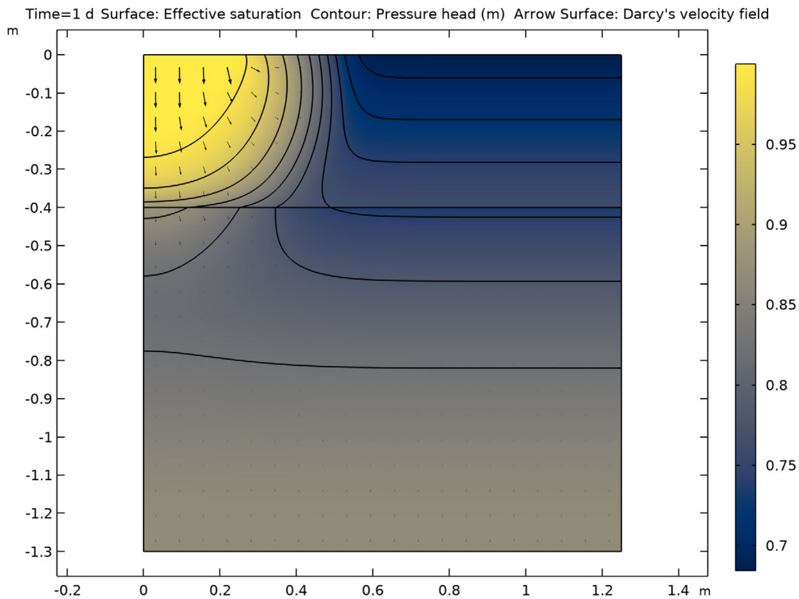


Figure 3: Estimates of effective saturation (surface plot), pressure head (contours), and velocity (arrows) in variably saturated soil after 1 day.

Figure 4 and Figure 5 give the concentrations for 0.3 days and 1 day, respectively, along with the retardation factor. They illustrate how the solute concentrations (surface plot) enter and move through the soil. Because the retardation factor depends on soil moisture, its value varies with the solution.

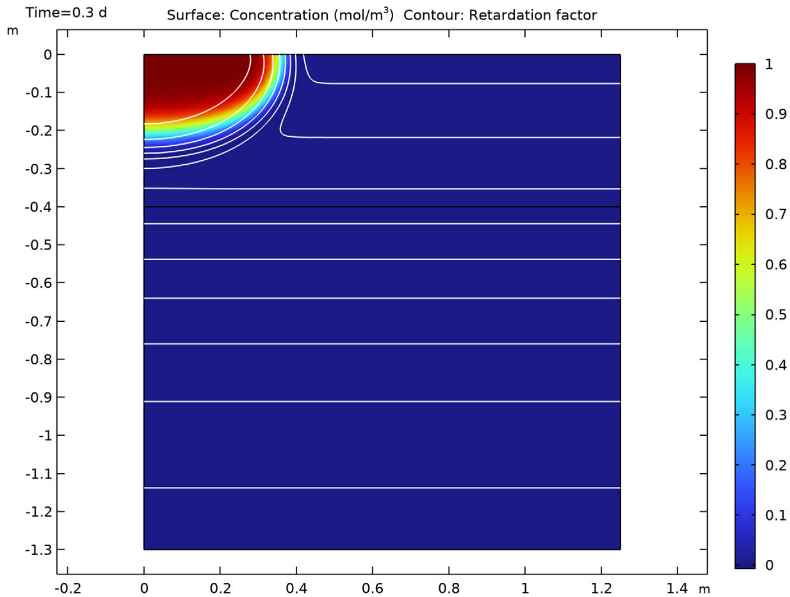


Figure 4: Solution for dissolved concentrations (surface plot) and retardation factor (contours) at 0.3 days.

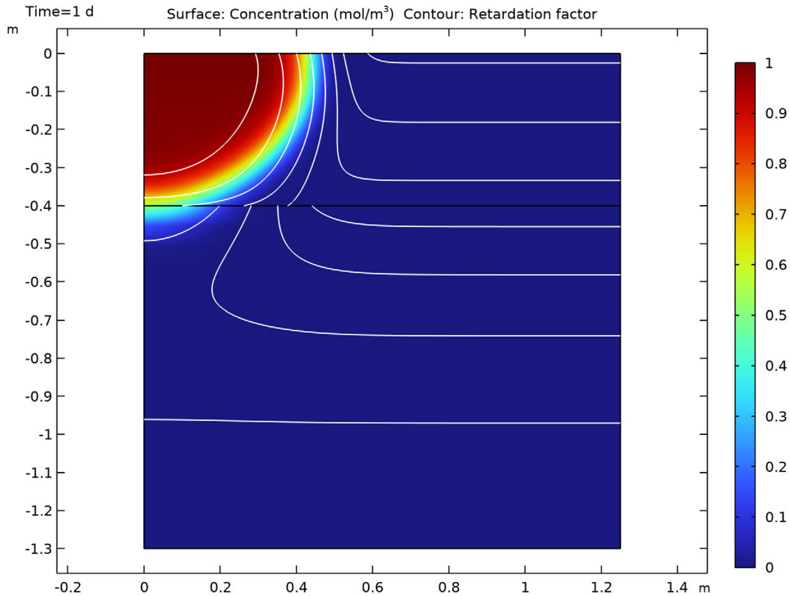


Figure 5: Solution for dissolved concentrations (surface plot) and retardation factor (contours) at 1 day.

Figure 6 shows an image of the retardation factor at the end of the simulation time interval. For variably saturated solute transport, the retardation factor changes with time. As shown in this image, the process of sorption has the greatest potential to slow the contaminant where the soils are relatively dry. The retardation coefficient here ranges from roughly 1.35 to 1.65, and the solute moves at approximately the velocity of the groundwater.

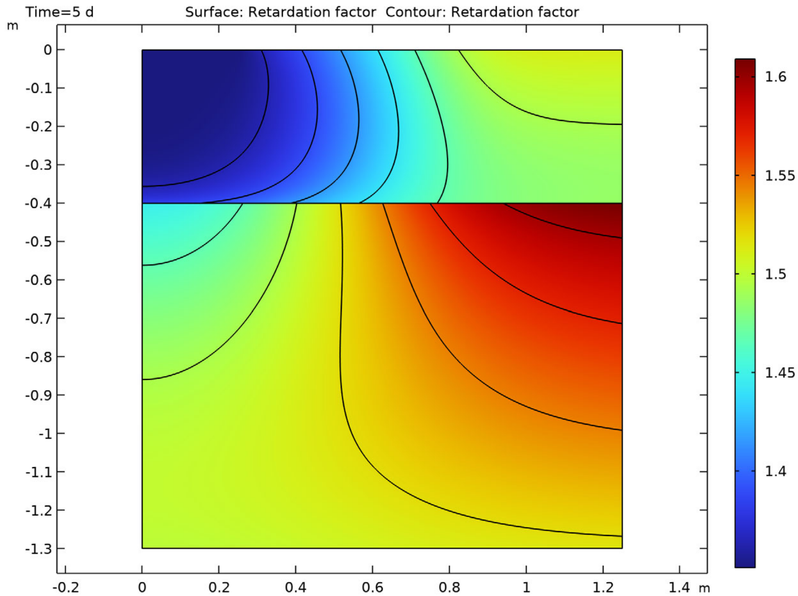


Figure 6: Snapshot of the retardation factor (surface and contours) at 5 days.

Notes About the COMSOL Implementation

This model makes use of the **Infinite Element Domain** feature. It performs a coordinate scaling to the selected domain such that boundary conditions on the 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. This allows to model details in an area which is actually very large or infinite.

References

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

2. 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.

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

4. J. Bear, *Hydraulics of Groundwater*, McGraw-Hill, 1978.

Application Library path: `Subsurface_Flow_Module/Solute_Transport/sorbing_solute`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow> Richards’ Equation (dl)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Chemical Species Transport> Transport of Diluted Species in Porous Media (tds)**.

5 Click **Add**.

6 Click **Study**.

7 In the **Select Study** tree, select **General Studies>Time Dependent**.

8 Click **Done**.

GLOBAL DEFINITIONS

Load the parameters from file.

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `sorbing_solute_parameters.txt`.

GEOMETRY 1

The modeling domain is made up of the two permeable soil layers, each of which is represented by a rectangular domain in 2D axisymmetry.

Rectangle 1 (r1)

1. In the **Geometry** toolbar, click **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `1.5`.
4. In the **Height** text field, type `0.9`.
5. Locate the **Position** section. In the **z** text field, type `-1.3`.
6. Click to expand the **Layers** section. Select the **Layers to the right** check box.
7. Clear the **Layers on bottom** check box.
8. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	0.25

This additional layer to the right will later be used to define an **Infinite Element Domain**. Read more about it in the Notes About the COMSOL Implementation section.

Proceed with the second soil layer.

Rectangle 2 (r2)

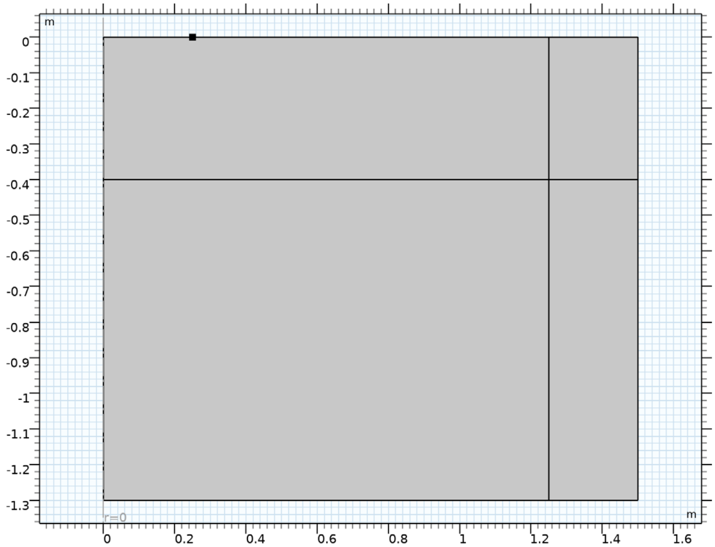
1. Right-click **Rectangle 1 (r1)** and choose **Duplicate**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Height** text field, type `0.4`.
4. Locate the **Position** section. In the **z** text field, type `-0.4`.

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

Point 1 (pt1)

1. In the **Geometry** toolbar, click **Point**.
2. In the **Settings** window for **Point**, locate the **Point** section.
3. In the **r** text field, type `0.25`.

4 Click **Build All Objects**.



Now, define the **Infinite Element Domain**.

DEFINITIONS

Infinite Element Domain 1 (ie1)

1 In the **Definitions** toolbar, click **Infinite Element Domain**.

2 Select Domains 3 and 4 only.

3 In the **Settings** window for **Infinite Element Domain**, locate the **Geometry** section.

4 From the **Type** list, choose **Cylindrical**.

RICHARDS' EQUATION (DL)

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.

Unsaturated Porous Medium 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Richards' Equation (dl)** click **Unsaturated Porous Medium 1**.

2 In the **Settings** window for **Unsaturated Porous Medium**, locate the **Porous Medium** section.

3 From the **Storage model** list, choose **User defined**. In the S_p text field, type `Sp_1`.

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.
2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.
3 From the **Permeability model** list, choose **Hydraulic conductivity**.
4 In the K_s text field, type `Ks_1`.
5 Locate the **Retention Model** section. In the α text field, type `alpha_1`.
6 In the n text field, type `n_1`.
7 In the θ_r text field, type `thetar_1`.

Unsaturated Porous Medium 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Richards' Equation (dl)** right-click **Unsaturated Porous Medium 1** and choose **Duplicate**.
2 Select Domains 2 and 4 only.
3 In the **Settings** window for **Unsaturated Porous Medium**, locate the **Porous Medium** section.
4 In the S_p text field, type `Sp_2`.

Porous Matrix 1

1 In the **Model Builder** window, expand the **Unsaturated Porous Medium 2** node, then click **Porous Matrix 1**.
2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.
3 In the K_s text field, type `Ks_2`.
4 Locate the **Retention Model** section. In the α text field, type `alpha_2`.
5 In the n text field, type `n_2`.
6 In the θ_r text field, type `thetar_2`.

Gravity 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Richards' Equation (dl)** click **Gravity 1**.
2 In the **Settings** window for **Gravity**, locate the **Gravity** section.
3 From the **Specify** list, choose **Elevation**.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.
2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
3 Click the **Pressure head** button.

4 In the H_p text field, type `-(z+1.2)`.

Initial Values 2

1 Right-click **Component 1 (comp1)>Richards' Equation (dl)>Initial Values 1** and choose **Duplicate**.

2 Select Domains 2 and 4 only.

3 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

4 In the H_p text field, type `-(z+1.2)-0.2*(z+0.4)`.

Pressure Head 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Pressure Head**.

2 Select Boundary 5 only.

3 In the **Settings** window for **Pressure Head**, locate the **Pressure Head** section.

4 In the H_{p0} text field, type `Hp0`.

Pervious Layer 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Pervious Layer**.

2 Select Boundaries 2 and 8 only.

3 In the **Settings** window for **Pervious Layer**, locate the **Pervious Layer** section.

4 In the H_b text field, type `-2`.

5 In the R_b text field, type `1/5[d]`.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Now, set up the transport equation for an unsaturated porous medium, accounting for dispersion and adsorption.

In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species in Porous Media (tds)**.

Unsaturated Porous Medium 1

1 In the **Physics** toolbar, click **Domains** and choose **Unsaturated Porous Medium**.

2 In the **Settings** window for **Unsaturated Porous Medium**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

Liquid 1

1 In the **Model Builder** window, click **Liquid 1**.

2 In the **Settings** window for **Liquid**, locate the **Saturation** section.

3 From the list, choose **Liquid volume fraction**.

4 In the θ_l text field, type `dl.theta_l`.

This corresponds to the liquid volume fraction.

5 From the **Liquid fraction time change** list, choose **Time change in pressure head**.

6 From the dH_p/dt list, choose **Time change in pressure head (dl)**.

7 In the C_m text field, type `dl.Cm`.

8 Locate the **Convection** section. From the **u** list, choose **Darcy's velocity field (dl)**.

9 Locate the **Diffusion** section. In the $D_{L,c}$ text field, type `Dl`.

Add adsorption as a subnode to the **Unsaturated Porous Medium** node.

Unsaturated Porous Medium 1

In the **Model Builder** window, click **Unsaturated Porous Medium 1**.

Adsorption 1

1 In the **Physics** toolbar, click **Attributes** and choose **Adsorption**.

2 In the **Settings** window for **Adsorption**, locate the **Adsorption** section.

3 From the **Adsorption isotherm** list, choose **User defined**.

4 Select the **Species c** check box.

5 In the $c_{P,c}$ text field, type `kp*c`.

Similarly, add dispersion as a subnode to the **Unsaturated Porous Medium** node.

Unsaturated Porous Medium 1

In the **Model Builder** window, click **Unsaturated Porous Medium 1**.

Dispersion 1

1 In the **Physics** toolbar, click **Attributes** and choose **Dispersion**.

2 In the **Settings** window for **Dispersion**, locate the **Dispersion** section.

3 From the **Dispersion tensor** list, choose **Dispersivity**.

4 From the **Dispersivity model** list, choose **Transverse isotropic**.

5 In the α table, enter the following settings:

alphar
alphaz

Reactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Reactions**.

2 In the **Settings** window for **Reactions**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Reaction Rates** section. In the R_c text field, type `(phip*kp*rhob-phil*dl.theta_l)*c`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundaries 2, 8, 12, and 13 only.

Concentration 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Concentration**.

2 Select Boundary 5 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species c** check box.

5 In the $c_{0,c}$ text field, type `c0`.

MATERIALS

Some required material properties have not yet been defined. This is indicated by a small red cross at the material node. Continue as follows to add the missing properties.

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.

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

Fluid 1 (pmat1.fluid1)

1 In the **Model Builder** window, click **Fluid 1 (pmat1.fluid1)**.

2 In the **Settings** window for **Fluid**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	rhof	kg/m³	Basic

Solid 1 (pmat1.solid1)

1 In the **Model Builder** window, click **Solid 1 (pmat1.solid1)**.

2 In the **Settings** window for **Solid**, locate the **Solid Properties** section.

3 In the θ_s text field, type `1-poro_1`.

4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	`rhob`	kg/m³	Basic

Porous Material: Upper Layer

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** right-click **Porous Material: Lower Layer (pmat1)** and choose **Duplicate**.

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

3 Select Domains 2 and 4 only.

Solid 1 (pmat2.solid1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials> Porous Material: Upper Layer (pmat2)** node, then click **Solid 1 (pmat2.solid1)**.

2 In the **Settings** window for **Solid**, locate the **Solid Properties** section.

3 In the θ_s text field, type `1-poro_2`.

MESH 1

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** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Finer**.

Mapped 1

In the **Mesh** toolbar, click **Mapped**.

Size 1

1 Right-click **Mapped 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

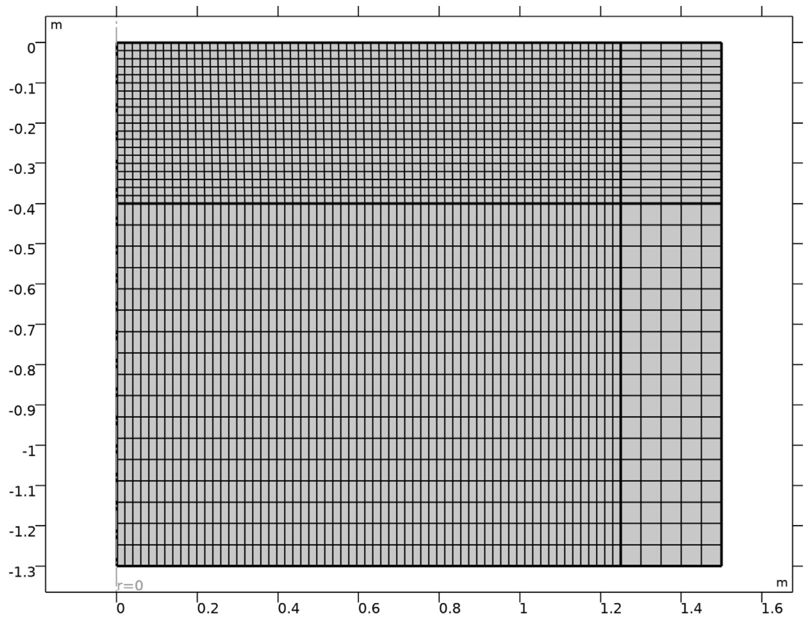
4 Select Domain 2 only.

5 Locate 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 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.



STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 From the **Time unit** list, choose **d**.

4 In the **Output times** text field, type `range(0,0.1,0.9) range(1,1,5)`.

5 In the **Home** toolbar, click **Compute**.

RESULTS

Study 1/Solution 1 (sol1)

Flownet, pressure and concentration plots are created per default. Pressure and concentration are also visualized on a revolved 3D geometry. Visualizing the results on the infinite element domains does not add value to the plots. Focus on the region close to the source and therefore hide the infinite element domains from the plots with the following steps.

In the **Model Builder** window, expand the **Results>Datasets** node, then click **Study 1/ Solution 1 (sol1)**.

Selection

1 In the **Results** toolbar, click **Attributes** and choose **Selection**.

2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domains 1 and 2 only.

The fourth default plot shows the solute concentration in the revolved geometry. Follow the steps below to reproduce the plots shown in Figure 4 and Figure 5.

Concentration (tds)

1 In the **Model Builder** window, under **Results** click **Concentration (tds)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Time (d)** list, choose **0.3**.

Contour 1

1 Right-click **Concentration (tds)** and choose **Contour**.

2 In the **Settings** window for **Contour**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Diluted Species in Porous Media>Species c>tds.RF_c - Retardation factor**.

3 Click to expand the **Title** section. From the **Title type** list, choose **Custom**.

4 Find the **Type and data** subsection. Clear the **Unit** check box.

5 Locate the **Levels** section. In the **Total levels** text field, type 10.

6 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

7 From the **Color** list, choose **White**.

8 Clear the **Color legend** check box.

9 Click to expand the **Quality** section. From the **Resolution** list, choose **Fine**.

Streamline 1

In the **Model Builder** window, right-click **Streamline 1** and choose **Disable**.

Concentration (tds)

1 In the **Model Builder** window, click **Concentration (tds)**.

2 In the **Concentration (tds)** toolbar, click **Plot**.

Compare the result with that in Figure 4.

3 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

4 From the **Time (d)** list, choose **1**.

5 In the **Concentration (tds)** toolbar, click **Plot**.

Compare with Figure 5.

Now plot the retardation factor after 5 days (Figure 6).

Retardation factor

1 Right-click **Concentration (tds)** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Retardation factor` in the **Label** text field.

3 Locate the **Data** section. From the **Time (d)** list, choose **5**.

Surface 1

1 In the **Model Builder** window, expand the **Retardation factor** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Transport of Diluted Species in Porous Media>Species c>tds.RF_c - Retardation factor**.

3 Click to expand the **Title** section. From the **Title type** list, choose **Custom**.

4 Find the **Type and data** subsection. Clear the **Unit** check box.

Contour 1

1 In the **Model Builder** window, click **Contour 1**.

2 In the **Settings** window for **Contour**, locate the **Coloring and Style** section.

3 From the **Color** list, choose **Black**.

4 In the **Retardation factor** toolbar, click **Plot**.

Proceed as follows to show the effective saturation, pressure head, and velocity field at different times.

2D Plot Group 7

In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

Surface 1

Right-click **2D Plot Group 7** and choose **Surface**.

Effective saturation

1 In the **Settings** window for **2D Plot Group**, type `Effective saturation` in the **Label** text field.

2 Locate the **Data** section. From the **Time (d)** list, choose **0.3**.

Surface 1

1 In the **Model Builder** window, click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Richards' Equation>Retention model>dl.Se - Effective saturation**.

3 Locate the **Title** section. From the **Title type** list, choose **Custom**.

4 Find the **Type and data** subsection. Clear the **Unit** check box.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Cividis**.

Contour 1

1 In the **Model Builder** window, right-click **Effective saturation** and choose **Contour**.

2 In the **Settings** window for **Contour**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Richards' Equation>Velocity and pressure>dl.Hp - Pressure head - m**.

3 Locate the **Levels** section. In the **Total levels** text field, type 10.

4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

5 From the **Color** list, choose **Black**.

6 Clear the **Color legend** check box.

Arrow Surface 1

1 Right-click **Effective saturation** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, locate the **Coloring and Style** section.

3 From the **Color** list, choose **Black**.

4 Locate the **Arrow Positioning** section. Find the **R grid points** subsection. In the **Points** text field, type 20.

5 Find the **Z grid points** subsection. In the **Points** text field, type 20.

6 In the **Effective saturation** toolbar, click **Plot**.

Compare the plot in the **Graphics** window with that in Figure 2.