

Pesticide Transport and Reaction in Soil

Introduction

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

This example looks at the degradation kinetics of aldicarb and its toxic by-products, investigating both the degradation time-scale as well as the spatial concentration distribution of toxic components. In the first model the chemicals are contained in a water pond, treated as a perfectly mixed system. The second model tracks the detailed distribution of chemicals in soil as the pesticide leaches out of the pond and is transported in water through the ground.

Model Definition

Aldicarb degrades by transformation to the corresponding sulfoxide and the sulfone (both of which are toxic), and is detoxified by hydrolysis to oximes and nitriles. The chain of reactions is illustrated in [Figure 1](#). The toxicity of a chemical species is indicated by its LD₅₀ value, signifying the median lethal dose (mg/kg) to half of a test population of rats. As indicated, both the sulfoxide and sulfone analogues of aldicarb are also relatively toxic.

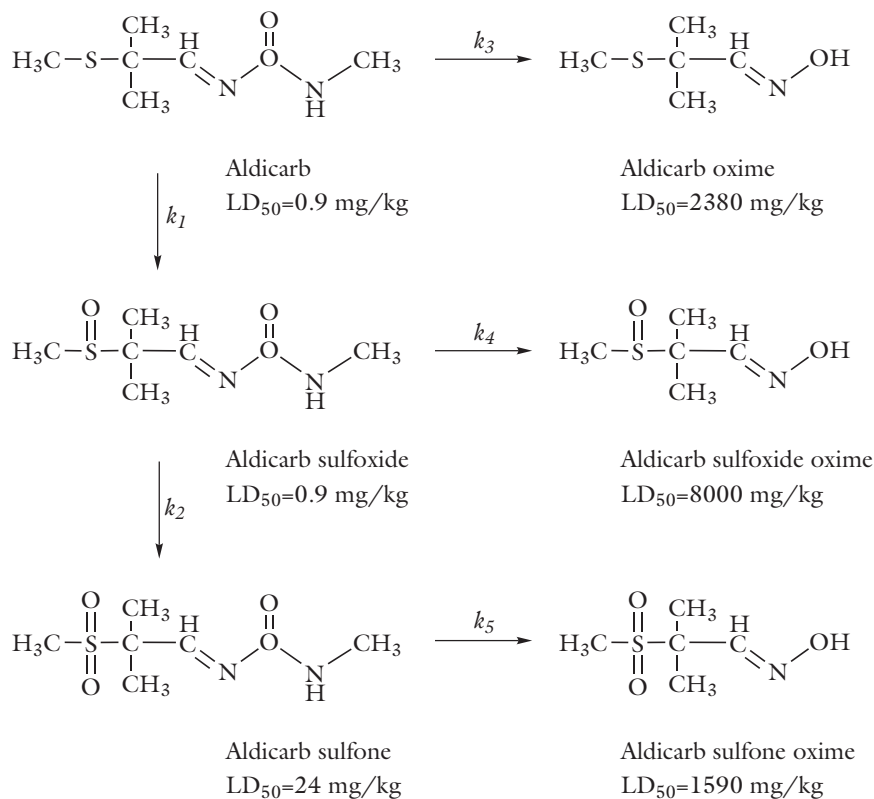


Figure 1: Reaction pathways of aldicarb degradation.

Each of the j unimolecular reactions outlined above has a rate expression of the form

$$r_j = k_j c_i$$

Note that in this example the concentration unit is kg/m^3 and the rate constants are expressed in $1/\text{day}$.

PERFECTLY MIXED SYSTEM

The first model solves for the decomposition kinetics of aldicarb occurring in a water pond. The pond is treated as a closed and perfectly mixed system. The reaction mechanism illustrated in Figure 1 translates into the following mass balance equations:

- For aldicarb (a)

$$\frac{dc_a}{dt} = -r_1 - r_3$$

- For aldicarb sulfoxide (asx)

$$\frac{dc_{asx}}{dt} = r_1 - r_2 - r_4$$

- For aldicarb sulfone (asn)

$$\frac{dc_{asn}}{dt} = r_2 - r_5$$

- For aldicarb oxime (ao)

$$\frac{dc_{ao}}{dt} = r_3$$

- For aldicarb sulfoxide oxime (asxo)

$$\frac{dc_{asxo}}{dt} = r_4$$

- For aldicarb sulfone oxime (asno)

$$\frac{dc_{asno}}{dt} = r_5$$

Solving this set of coupled ODEs provides information on the time scales of the degradation processes.

SPACE- AND TIME-DEPENDENT SYSTEM

In a more detailed model, assume that aldicarb moves from the pond into relatively dry soil. In the soil, the aldicarb decomposes according to the mechanism illustrated in [Figure 1](#). In addition, the pesticide and its decay products are transported by advection, dispersion, sorption, and volatilization.

Geometry

Water is ponded by a ring sitting on the ground. The soil is layered and rests on rocks, with the top layer slightly less permeable than the bottom one. 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 surface outside of the ring.

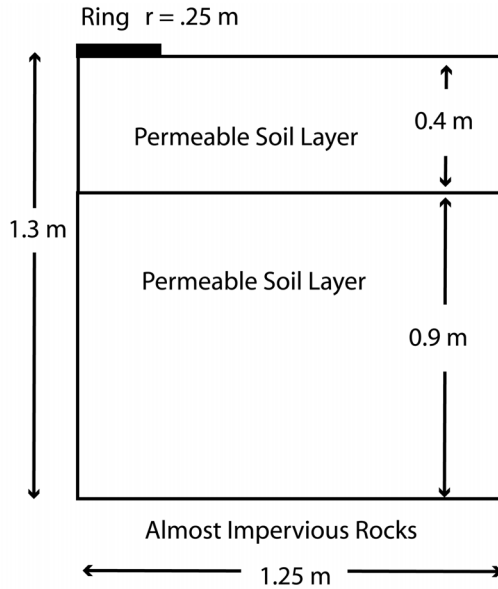


Figure 2: Geometry of the infiltration ring and soil column.

Aldicarb moves with water from the pond into the soil at a constant concentration. In the soil, the chemicals react and also sorb onto soil particles. Aldicarb and the aldicarb sulfone volatilize to the atmosphere. The sorption, biodegradation, and volatilization proceed in linear proportion to the aqueous concentrations. The soil is initially pristine with zero concentration of the involved chemicals. At the ground surface outside the ring there is volatilization to the atmosphere for c_a and c_{asn} . The vertical axis is a line of symmetry. The other boundaries are posed such that the solutes can freely leave the soil column with the fluid flow. Model the problem with 2D axisymmetry and track the solute transport for 10 days.

Fluid Flow

Richards' equation governs the saturated-unsaturated flow of water in 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 use Richards' equation for single-phase flow. Given by [Ref. 1](#), Richards' equation in pressure head reads

$$(C + SeS)\frac{\partial H_p}{\partial t} + \nabla \cdot (-K\nabla(H_p + D)) = 0$$

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

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

Also, the permeability κ (SI unit: $1/\text{m}^2$) 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, $S = (\theta_s - \theta_r)/(1 \text{ m} \cdot \rho g)$ 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*.

Mass Transport

The governing equation for solute transport describes advection and dispersion of a sorbing, volatilizing, and decaying solute in variably saturated soil.

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_b c_p) + \nabla \cdot (-\theta D_L \nabla c + \mathbf{u}c) = \Sigma R_L + \Sigma R_P + S_c \quad (1)$$

The Solute Transport interface implements [Equation 1](#). It describes the time rate of change in two terms: c denotes dissolved concentration (kg/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 (dimensionless), and ρ_b is the bulk density (kg/m^3). Because ρ_b amounts to the dried solid mass per bulk volume of the solids and pores together, the term $\rho_b c_p$ gives solute mass attached to the soil as the concentration changes with time.

Solute spreading now includes mechanical dispersion in water plus molecular diffusion for water and air. These three processes appear in the liquid-gas dispersion tensor, whose entries are

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

$$\theta D_{LGij} = \theta D_{LGji} = (\alpha_1 - \alpha_2) \frac{u_i u_j}{|\mathbf{u}|} \quad (3)$$

In these equations, D_{LGii} are the principal components of the liquid-gas dispersion tensor; D_{LGij} and D_{LGji} are the cross terms; α is the dispersivity (m) where the subscripts “1” and “2” denote longitudinal and transverse flow, respectively; D_m and D_G (m^2/d) are molecular diffusion coefficients; and τ_L and τ_G give the tortuosity factors for liquid (water) and gas (air), respectively.

The three solutes—aldicarb, aldicarb sulfoxide, and aldicarb sulfone—have different decay terms, R_{Li} , partition coefficients, k_{pi} , and volatilization constants, k_{Gi} . All of the solutes attach to soil particles. Two of the solutes volatilize; sulfoxide does not.

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
H_{p0}	m	Pressure head in ring	0.01	
$H_{p,\text{init}}$	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

VARIABLE	UNITS	DESCRIPTION	VALUE
α_z	m	Transverse dispersivity	0.001
ϕ_L	d ⁻¹	Decay rate in liquid	0.05
ϕ_P	d ⁻¹	Decay rate on solid	0.01
c_0	kg/m ³	Solute concentration in ring	1.0
c_{init}	kg/m ³	Initial solute concentration in soil	0

Results and Discussion

First, review the results of the perfectly mixed reactor model. [Figure 3](#) shows the concentration profiles of aldicarb and all of its decay products. Only small amounts of aldicarb remain after 10 days. [Figure 4](#) shows the concentration transients of the three most toxic species—aldicarb, aldicarb sulfoxide, and aldicarb sulfone—as well as their sum (see [Figure 1](#) for LD₅₀ values). Considering the summed-up contributions, contamination levels clearly remain high even after several months.

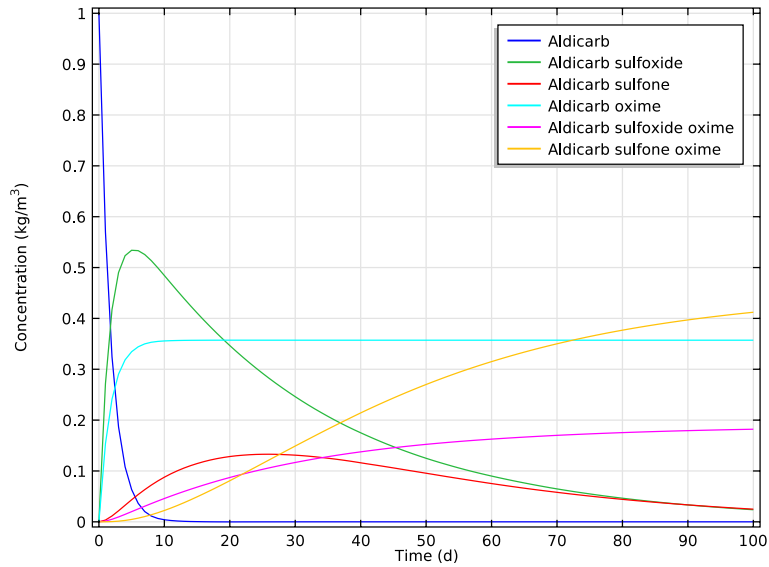


Figure 3: Concentration profiles as reactions occur during a 100 day time period.

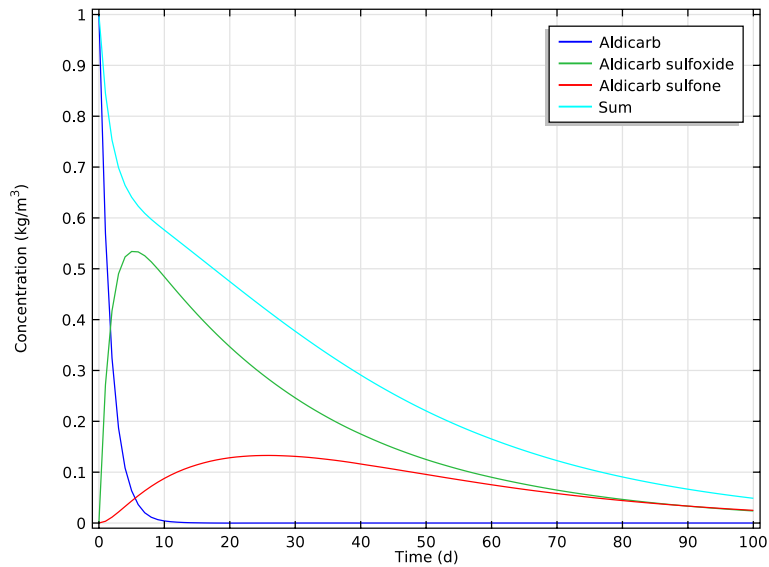


Figure 4: Concentration transients of the most toxic species, aldicarb (c_a), aldicarb sulfoxide (c_{asx}), and aldicarb sulfone (c_{asn}).

The following results come from the space- and time-dependent model setup. Figure 5 shows the fluid flow in soil after 0.3 days (left) and 1.0 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.

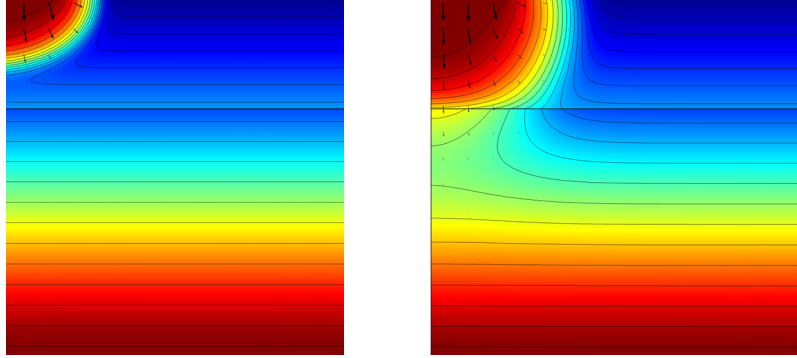


Figure 5: The effective saturation (surface plot), pressure head (contours), and flow velocity (arrows) in a variably saturated soil after 0.3 days (left) and 1 day (right).

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.

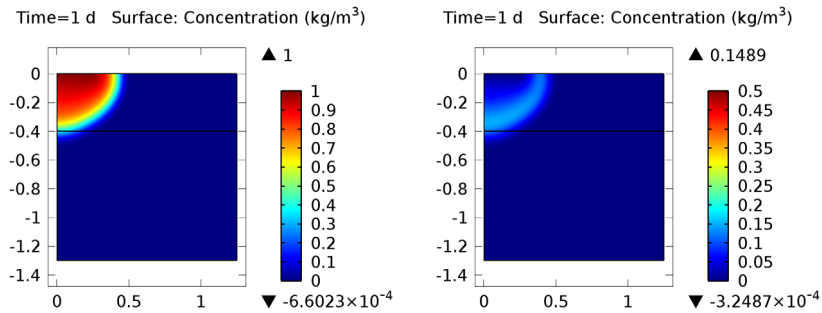


Figure 6: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 1 day (note the differing color ranges).

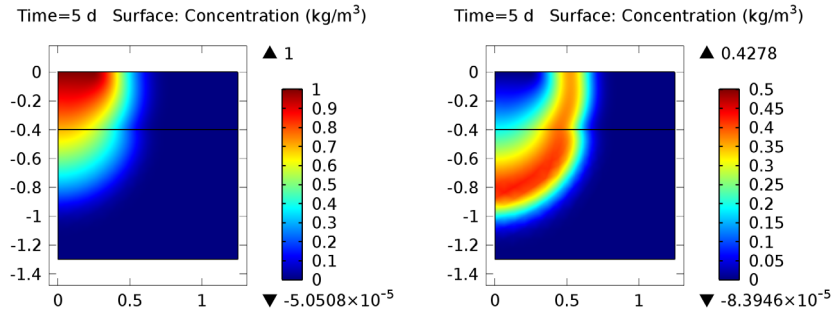


Figure 7: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 5 days.

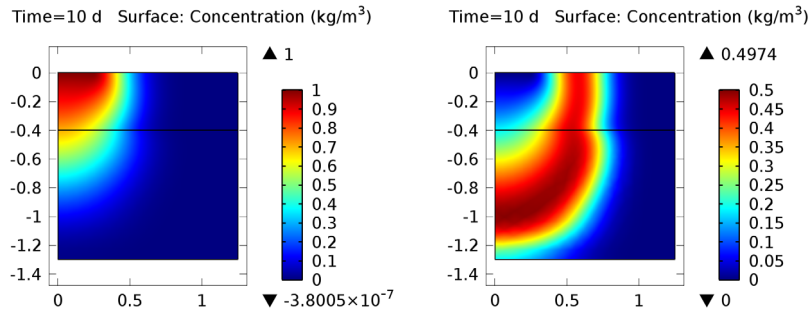


Figure 8: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 10 days.

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 4). 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, 1978.
2. M.Th. van Genuchten, "A closed-form equation for predicting the hydraulic of conductivity of unsaturated soils," *Soil Sci. Soc. Am. J.*, vol. 44, pp. 892–898, 1980.

Model Library path: Subsurface_Flow_Module/Solute_Transport/
pesticide_transport

Modeling Instructions

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

NEW

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

MODEL WIZARD

- 1** In the **Model Wizard** window, click the **2D Axisymmetric** button.
- 2** In the **Select physics** tree, select **Mathematics>ODE and DAE Interfaces>Global ODEs and DAEs (ge)**.
- 3** Click the **Add** button.
- 4** Click the **Study** button.
- 5** In the tree, select **Preset Studies>Time Dependent**.
- 6** Click the **Done** button.

GLOBAL DEFINITIONS

Load the rate constants from file.

Parameters

- 1** On the **Home** toolbar, click **Parameters**.
- 2** In the **Parameters** settings window, locate the **Parameters** section.
- 3** Click **Load from File**.
- 4** Browse to the model's Model Library folder and double-click the file
pesticide_transport_parameters_1.txt.
First consider the aldicarb decomposition kinetics in the the water pond treated as
a perfectly mixed system.

GLOBAL ODES AND DAES (GE)

Global Equations 1

Read in a set of the equations defining the reactions.

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Global ODEs and DAEs (ge)** click **Global Equations 1**.
- 2 In the **Global Equations** settings window, locate the **Global Equations** section.
- 3 Click **Load from File**.
- 4 Browse to the model's Model Library folder and double-click the file `pesticide_transport_reactions.txt`.

STUDY 1

Step 1: Time Dependent

- 1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.
- 2 In the **Time Dependent** settings window, locate the **Study Settings** section.
- 3 From the **Time unit** list, choose **d**.
- 4 In the **Times** edit field, type range (0, 1, 100).
- 5 On the **Home** toolbar, click **Compute**.

RESULTS

ID Plot Group 1

Reproduce [Figure 3](#) with the following steps:

- 1 In the **ID Plot Group** settings window, click to expand the **Title** section.
- 2 From the **Title type** list, choose **None**.
- 3 Locate the **Plot Settings** section. Select the **y-axis label** check box.
- 4 In the associated edit field, type Concentration (kg/m³).
- 5 In the **Model Builder** window, expand the **ID Plot Group 1** node, then click **Global 1**.
- 6 In the **Global** settings window, locate the **x-Axis Data** section.
- 7 From the **Parameter** list, choose **Expression**.
- 8 In the **Expression** edit field, type `t`.
- 9 From the **Unit** list, choose **d**.
- 10 On the **ID plot group** toolbar, click **Plot**.

To plot the concentration of the most toxic species, as in [Figure 4](#), proceed as follows:

ID Plot Group 2

- 1 In the **Model Builder** window, right-click **ID Plot Group 1** and choose **Duplicate**.

2 In the **Model Builder** window, expand **ID Plot Group 2** and click **Global 1**.

Delete the expressions **cpm_ao**, **cpm_asno**, and **cpm_asxo**.

3 In the table, enter the following settings:

Expression	Unit	Description
cpm_a		Aldicarb
cpm_asx		Aldicarb sulfoxide
cpm_asn		Aldicarb sulfone
cpm_a+cpm_asn+cpm_asx		Sum

4 On the **ID plot group** toolbar, click **Plot**.

Now solve the time- and space-dependent transport and reaction problem in the soil.

COMPONENT 1 (COMPI)

On the **Home** toolbar, click **Add Physics**.

ADD PHYSICS

1 Go to the **Add Physics** window.

2 In the **Add physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow>Richards' Equation (dl)**.

3 Find the **Physics in study** subsection. In the table, enter the following settings:

Studies	Solve
Study I	×

4 In the **Add physics** window, click **Add to Component**.

ADD PHYSICS

1 Go to the **Add Physics** window.

2 In the **Add physics** tree, select **Chemical Species Transport>Solute Transport (esst)**.

3 Click to expand the **Dependent variables** section. Locate the **Dependent Variables** section. In the **Number of species** edit field, type 3.

4 In the **Concentrations** table, enter the following settings:

c_a
c_asx
c_asn

5 Find the **Physics in study** subsection. In the table, enter the following settings:

Studies	Solve
Study I	×

6 In the **Add physics** window, click **Add to Component**.

ROOT

On the **Home** toolbar, click **Add Study**.

ADD STUDY

1 Go to the **Add Study** window.

2 Find the **Physics in study** subsection. In the table, enter the following settings:

Physics	Solve
Global ODEs and DAEs (ge)	×

3 Find the **Studies** subsection. In the tree, select **Preset Studies>Time Dependent**.

4 In the **Add study** window, click **Add Study**.

Load the parameters defining the material properties and the geometry from file.

GLOBAL DEFINITIONS

Parameters

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

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `pesticide_transport_parameters_2.txt`.

GEOMETRY I

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 **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type 1.25.

- 4 In the **Height** edit field, type 0.9.
- 5 Locate the **Position** section. In the **z** edit field, type -1.3.
- 6 Click the **Build Selected** button.

Rectangle 2 (r2)

- 1 In the **Model Builder** window, right-click **Geometry 1** and choose **Rectangle**.
- 2 In the **Rectangle** settings window, locate the **Size** section.
- 3 In the **Width** edit field, type 1.25.
- 4 In the **Height** edit field, type 0.4.
- 5 Locate the **Position** section. In the **z** edit field, type -0.4.
- 6 Click the **Build Selected** button.
- 7 Click the **Zoom Extents** button on the Graphics toolbar.

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

Point 1 (pt1)

- 1 Right-click **Geometry 1** and choose **Point**.
- 2 In the **Point** settings window, locate the **Point** section.
- 3 In the **r** edit field, type 0.25.
- 4 Click the **Build All Objects** button.



DEFINITIONS

Variables 1a

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

Load the rate expressions from file.

- 2 In the **Variables** settings window, locate the **Variables** section.
- 3 Click **Load from File**.
- 4 Browse to the model's Model Library folder and double-click the file `pesticide_transport_variables.txt`.

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.

Richards' Equation Model 1

- 1 In the **Model Builder** window, expand the **Richards' Equation (dl)** node, then click **Richards' Equation Model 1**.
- 2 In the **Richards' Equation Model** settings window, locate the **Fluid Properties** section.
- 3 From the ρ list, choose **User defined**. In the associated edit field, type ρ .
- 4 Locate the **Matrix Properties** section. From the **Permeability model** list, choose **Hydraulic conductivity**.
- 5 In the K_s edit field, type Ks_1 .
- 6 In the θ_s edit field, type $\thetaetas_1$.
- 7 In the θ_r edit field, type $\thetaetar_1$.
- 8 Locate the **Storage Model** section. From the S list, choose **User defined**. In the **Storage** edit field, type Ss_1 .
- 9 Locate the **Retention Model** section. In the α edit field, type α_1 .
- 10 In the n edit field, type n_1 .

Richards' Equation Model 2

- 1 Right-click **Component 1 (comp1)**>**Richards' Equation (dl)**>**Richards' Equation Model 1** and choose **Duplicate**.
- 2 Select Domain 2 only.
- 3 In the **Richards' Equation Model** settings window, locate the **Matrix Properties** section.

- 4 In the K_s edit field, type Ks_2 .
- 5 In the θ_s edit field, type $thetas_2$.
- 6 In the θ_r edit field, type $thetar_2$.
- 7 Locate the **Storage Model** section. In the **Storage** edit field, type Ss_2 .
- 8 Locate the **Retention Model** section. In the α edit field, type $alpha_2$.
- 9 In the n edit field, type n_2 .

Initial Values 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Richards' Equation (dl)** click **Initial Values 1**.
- 2 In the **Initial Values** settings window, locate the **Initial Values** section.
- 3 Click the **Pressure head** button.
- 4 In the H_p edit 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 Domain 2 only.
- 3 In the **Initial Values** settings window, locate the **Initial Values** section.
- 4 In the H_p edit field, type $-(z+1.2) - 0.2*(z+0.4)$.

Pressure Head 1

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Pressure Head**.
- 2 Select Boundary 5 only.
- 3 In the **Pressure Head** settings window, locate the **Pressure Head** section.
- 4 In the H_{p0} edit field, type $Hp0$.

Mass Flux 1

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Mass Flux**.
- 2 Select Boundary 2 only.
- 3 In the **Mass Flux** settings window, locate the **Mass Flux** section.
- 4 In the N_0 edit field, type $-N0$.

SOLUTE TRANSPORT (ESST)

Mobile Liquid, Immobile Solid and Gas 1

- 1 Click **Component 1 (comp1)>Solute Transport**.

- 2 On the **Physics** toolbar, click **Domains** and choose **Mobile Liquid, Immobile Solid and Gas**.
- 3 In the **Mobile Liquid, Immobile Solid and Gas** settings window, locate the **Domain Selection** section.
- 4 From the **Selection** list, choose **All domains**.
- 5 Locate the **Model Inputs** section. From the **u** list, choose **Darcy's velocity field (dl)**.
- 6 Locate the **Porous Medium** section. In the θ_s edit field, type `dl.theta`.
- 7 In the θ edit field, type `dl.theta`.
These settings couple the solute transport to the flow calculated by the Richards' Equation interface.
- 8 In the ρ_b edit field, type `rhob`.
- 9 From the **Fluid fraction time change** list, choose **Time change in pressure head**.
- 10 From the dH_p/dt list, choose **Time change in pressure head (dl)**.
- 11 In the C_m edit field, type `dl.Cm`.
- 12 Click to expand the **Sorption** section. From the **Species c_a** list, choose **User defined**.
- 13 In the $k_{p,ca}$ edit field, type `kp_a`.
- 14 From the **Species c_asx** list, choose **User defined**.
- 15 In the $k_{p,casx}$ edit field, type `kp_asx`.
- 16 From the **Species c_asn** list, choose **User defined**.
- 17 In the $k_{p,casn}$ edit field, type `kp_asn`.
- 18 Click to expand the **Volatilization** section. In the $k_{G,ca}$ edit field, type `kg_a`.
- 19 In the $k_{G,casn}$ edit field, type `kg_asn`.
- 20 Click to expand the **Dispersion** section. Specify the α vector as

alphan	r
alphaz	z

- 21 Click to expand the **Diffusion** section. In the $D_{L,ca}$ edit field, type `Dl`.
- 22 In the $D_{L,casx}$ edit field, type `Dl`.
- 23 In the $D_{L,casn}$ edit field, type `Dl`.
- 24 In the $D_{G,ca}$ edit field, type `Dg`.
- 25 In the $D_{G,casx}$ edit field, type `Dg`.
- 26 In the $D_{G,casn}$ edit field, type `Dg`.

Reactions I

- 1 On the **Physics** toolbar, click **Domains** and choose **Reactions**.
- 2 In the **Reactions** settings window, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **Reactions** section. In the R_{ca} edit field, type $d1.\theta*(-r_1-r_3)$.
- 5 In the R_{casx} edit field, type $d1.\theta*(r_1-r_2-r_4)$.
- 6 In the R_{casn} edit field, type $d1.\theta*(r_2-r_5)$.

Outflow I

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
- 2 Select Boundaries 2, 7, and 8 only.

Concentration I

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Concentration**.
- 2 Select Boundary 5 only.
- 3 In the **Concentration** settings window, locate the **Concentration** section.
- 4 Select the **Species c_a** check box.
- 5 In the $c_{0,ca}$ edit field, type c_0 .
- 6 Select the **Species c_asx** check box.
- 7 Select the **Species c_asn** check box.

No Flow Boundary Volatilization I

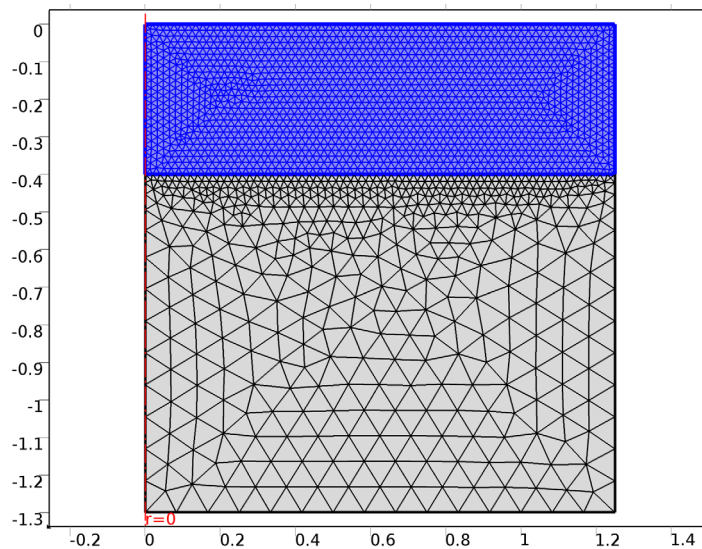
- 1 On the **Physics** toolbar, click **Boundaries** and choose **No Flow Boundary Volatilization**.
- 2 Select Boundary 6 only.
- 3 In the **No Flow Boundary Volatilization** settings window, locate the **No Flow Boundary Volatilization** section.
- 4 Select the **Species c_a** check box.
- 5 In the d_{ca} edit field, type d_a .
- 6 Select the **Species c_asn** check box.
- 7 In the d_{casn} edit field, type d_{asn} .

MESH I*Free Triangular I*

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Free Triangular**.

Size 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** right-click **Free Triangular 1** and choose **Size**.
- 2 In the **Size** settings window, 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 edit field, type 0.02.
- 8 Click the **Build All** button.

**STUDY 2***Step 1: Time Dependent*

- 1 In the **Model Builder** window, expand the **Study 2** node, then click **Step 1: Time Dependent**.
- 2 In the **Time Dependent** settings window, locate the **Study Settings** section.
- 3 From the **Time unit** list, choose **d**.
- 4 In the **Times** edit field, type `range(0,0.1,0.9) range(1,1,10)`.

- 5 Locate the **Physics and Variables Selection** section. In the table, make sure that the Global ODEs are not solved:

Physics	Solve for	Discretization
Global ODEs and DAEs	×	physics

- 6 On the **Home** toolbar, click **Compute**.

RESULTS

Pressure (dl)

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

- 1 In the **Model Builder** window, click **Pressure (dl)**.
- 2 In the **2D Plot Group** settings window, locate the **Data** section.
- 3 From the **Time (d)** list, choose **0.3**.
- 4 In the **Model Builder** window, expand the **Pressure (dl)** node, then click **Surface 1**.
- 5 In the **Surface** settings window, locate the **Expression** section.
- 6 Type **dl.Se**. Locate the **Coloring and Style** section. Clear the **Color legend** check box.
- 7 Click the **Zoom Extents** button on the Graphics toolbar.
- 8 In the **Model Builder** window, right-click **Pressure (dl)** and choose **Contour**.
- 9 In the **Contour** settings window, locate the **Expression** section.
- 10 Type **dl.Hp**. Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 11 From the **Color** list, choose **Black**.
- 12 Clear the **Color legend** check box.
- 13 Click to expand the **Quality** section. From the **Resolution** list, choose **Finer**.
- 14 Right-click **Pressure (dl)** and choose **Arrow Surface**.
- 15 In the **Arrow Surface** settings window, locate the **Coloring and Style** section.
- 16 From the **Color** list, choose **Black**.
- 17 On the **2D plot group** toolbar, click **Plot**.
Compare the plot in the Graphics window with that in the left panel of [Figure 5](#).
- 18 In the **Model Builder** window, click **Pressure (dl)**.
- 19 In the **2D Plot Group** settings window, locate the **Data** section.

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

21 On the **2D plot group** toolbar, click **Plot**.

Compare with the right panel of [Figure 5](#).

22 Right-click **Pressure (dl)** and choose **Rename**.

23 Go to the **Rename 2D Plot Group** dialog box and type **Effective saturation** in the **New name** edit field.

24 Click **OK**.

The third default plot shows the solute concentration at $t = 10$ days. Follow the steps below to reproduce the plots shown in [Figure 6--Figure 8](#).

Concentration (esst)

1 In the **Model Builder** window, expand the **Concentration (esst)** node, then click **Surface 1**.

2 In the **Surface** settings window, click to expand the **Range** section.

3 Select the **Manual color range** check box.

4 In the **Minimum** edit field, type **0**.

5 In the **Maximum** edit field, type **1**.

These settings give a single color range for all three aldicarb concentration plots.

6 Click to collapse the **Range** section. On the **2D plot group** toolbar, click **Plot**.

7 Click the **Zoom Extents** button on the Graphics toolbar.

8 In the **Model Builder** window, click **Concentration (esst)**.

9 In the **2D Plot Group** settings window, locate the **Data** section.

10 From the **Time (d)** list, choose **5**.

11 On the **2D plot group** toolbar, click **Plot**.

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

13 On the **2D plot group** toolbar, click **Plot**.

14 Right-click **Concentration (esst)** and choose **Rename**.

15 Go to the **Rename 2D Plot Group** dialog box and type **Concentration, aldicarb** in the **New name** edit field.

16 Click **OK**.

Concentration, aldicarb 1

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

- 2 In the **Model Builder** window, expand the **Concentration, aldicarb I** node, then click **Surface I**.
- 3 In the **Surface** settings window, locate the **Expression** section.
- 4 Click **Concentration (c_asx)** in the upper-right corner of the section. Click to expand the **Range** section. In the **Maximum** edit field, type 0.5.
Because the maximum concentration for aldicarb sulfoxide is lower, this setting makes better use of the color range.
- 5 Click to collapse the **Range** section. On the **2D plot group** toolbar, click **Plot**.
- 6 In the **Model Builder** window, click **Concentration, aldicarb I**.
- 7 In the **2D Plot Group** settings window, locate the **Data** section.
- 8 From the **Time (d)** list, choose **5**.
- 9 On the **2D plot group** toolbar, click **Plot**.
- 10 From the **Time (d)** list, choose **10**.
- 11 On the **2D plot group** toolbar, click **Plot**.
- 12 Right-click **Concentration, aldicarb I** and choose **Rename**.
- 13 Go to the **Rename 2D Plot Group** dialog box and type **Concentration, aldicarb sulfoxide** in the **New name** edit field.
- 14 Click **OK**.

You can also visualize the evolution of the concentration distributions with time through animations. By adding **Animation** features under the **Export** node, you can generate movies in GIF, Flash, and AVI format. Alternatively, add **Player** features with animations contained inside the model MPH-file as follows:

Concentration, aldicarb

In the **Model Builder** window, under **Results** click **Concentration, aldicarb**. Click the **Player** button on the **Results** toolbar.

Concentration, aldicarb sulfoxide

In the **Model Builder** window, under **Results** click **Concentration, aldicarb sulfoxide**. Click the **Player** button on the **Results** toolbar.

