



Model created in COMSOL Multiphysics 6.4

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.

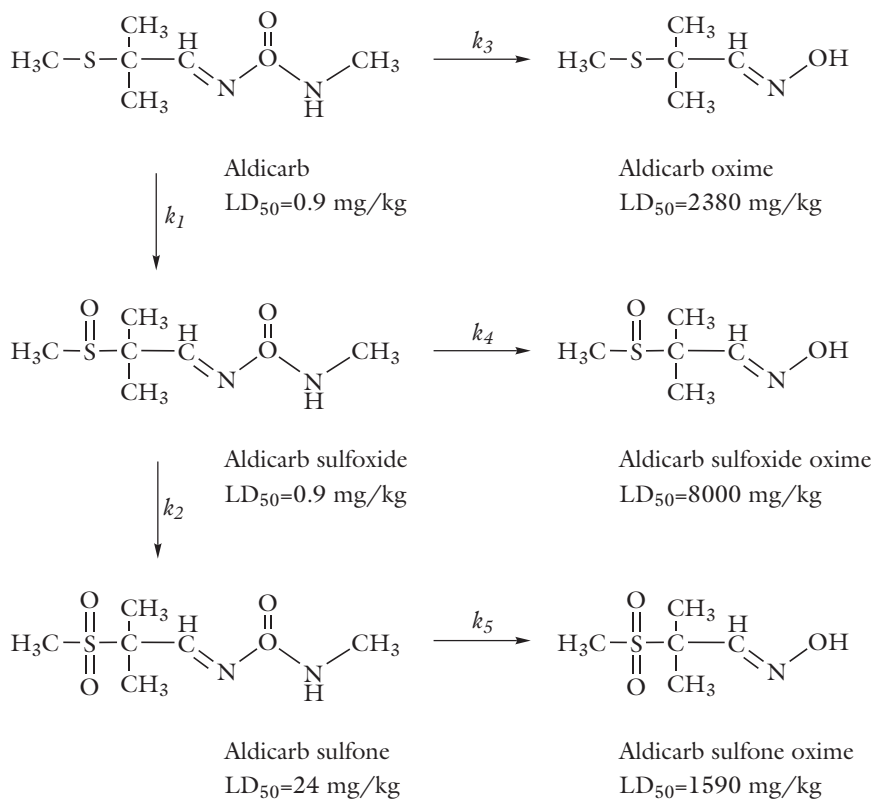


Figure 1: Reaction pathways of aldicarb degradation.

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 mol/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 convection, 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.

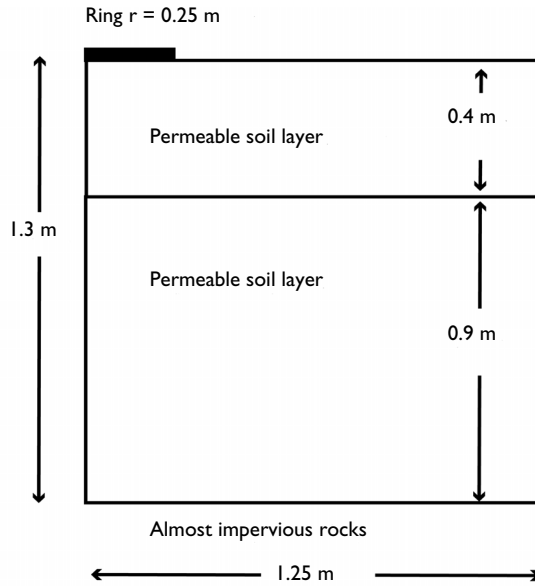


Figure 2: Geometry of the infiltration ring and soil column.

Aldicarb moves with water from the pond into the soil at a constant concentration. In the soil, the chemicals react and also adsorb 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} . Model the problem with 2D axisymmetry and track the solute transport for 10 days. The vertical axis to the left is the symmetry axis. Add infinite elements to the right axis such that the solutes can freely leave the soil column with the fluid flow.

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

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

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); 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: $1/m^2$) 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, $S_p = (\theta_s - \theta_r)/(1 \text{ m} \cdot \rho g)$ 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.

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

The Transport of Diluted Species in Porous Media interface implements [Equation 1](#). It describes the 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 fraction of fluid (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 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

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

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

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 dispersivities, 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 adsorb to soil particles, but only 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

VARIABLE	UNITS	DESCRIPTION	VALUE
α_r	m	Longitudinal dispersivity	0.005
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	mol/m ³	Solute concentration in ring	1.0

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 as well as the sum of the three most toxic species — aldicarb, aldicarb sulfoxide, and aldicarb sulfone (see Figure 1 for LD₅₀ values). Only small amounts of aldicarb remain after 10 days. Considering the summed-up contributions, contamination levels clearly remain high even after several months.

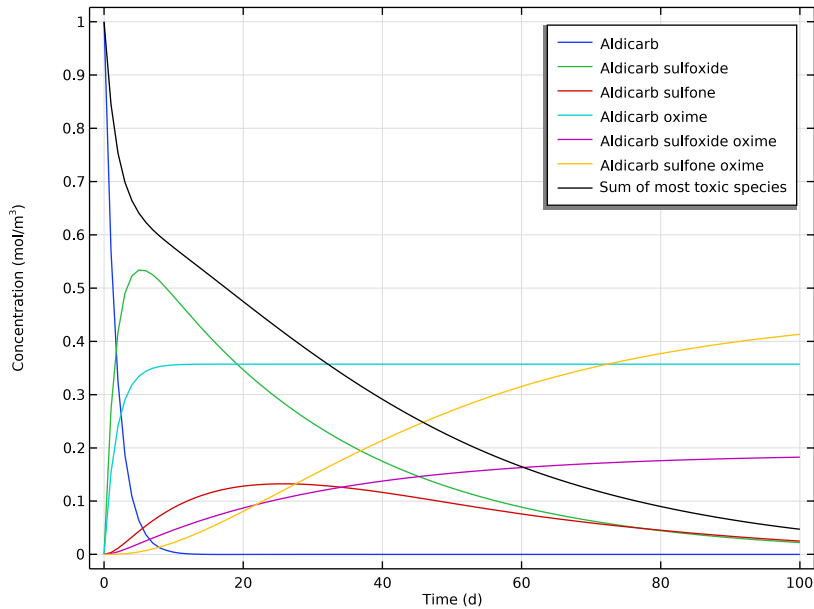


Figure 3: Concentration profiles as reactions occur during a 100 day time period.

The following results come from the space- and time-dependent model setup. Figure 4 shows the Pressure Head distribution after 10 days

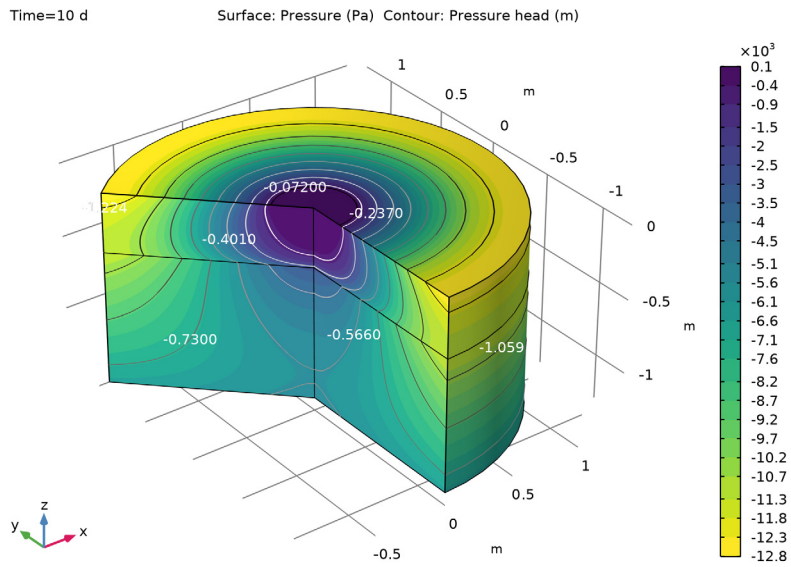


Figure 4: Pressure head after 10 days.

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.

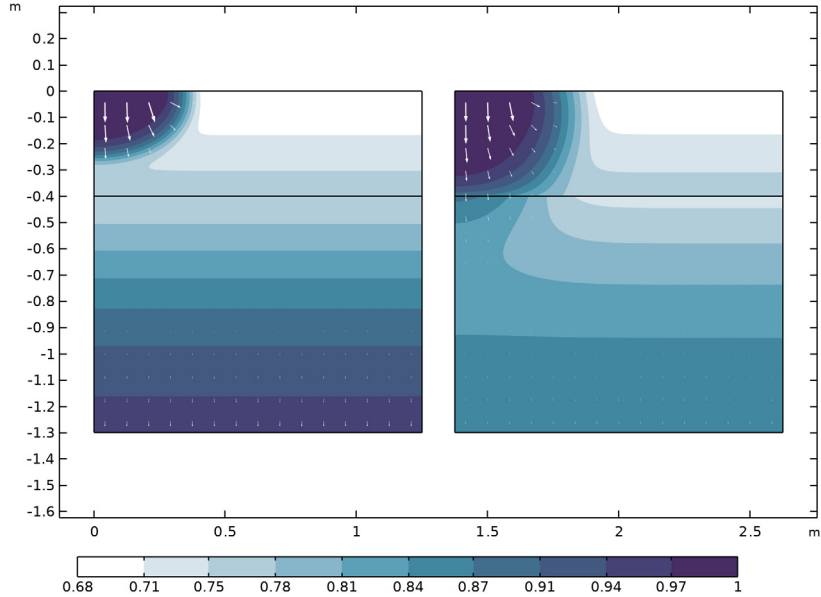


Figure 5: The effective saturation (surface plot), and flow velocity (arrows) in a variably saturated soil after 0.3 days (left) and 1 day (right).

Figure 6 shows 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.

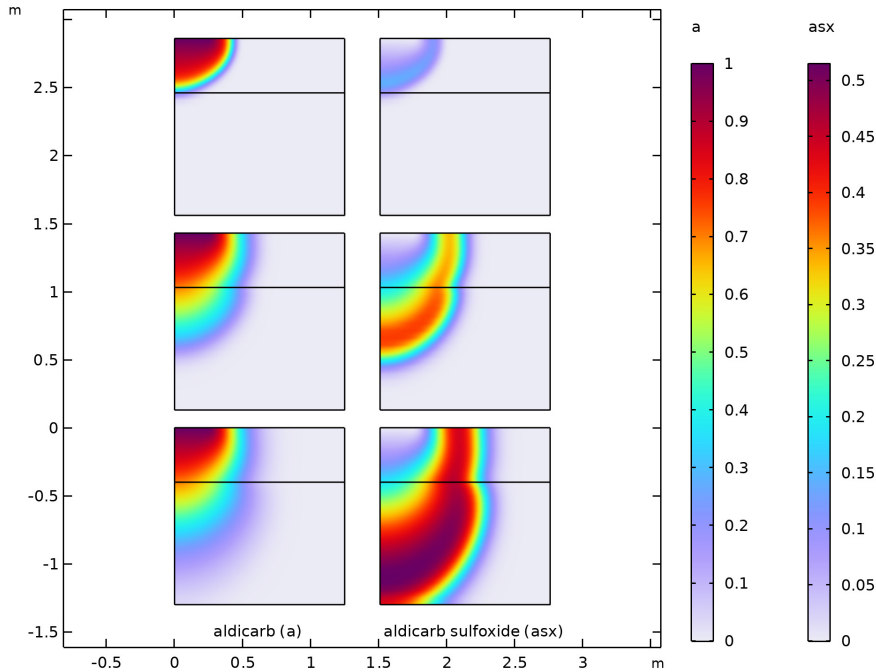


Figure 6: Concentration of aldicarb (left) and aldicarb sulfoxide (right) after 1, 5, and 10 days (note the differing color ranges).

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 3). 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.

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. 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.

Application Library path: Subsurface_Flow_Module/Solute_Transport/
pesticide_transport




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 **Mathematics > ODE and DAE Interfaces > Global ODEs and DAEs (ge)**.
- 3 Click **Add**.
- 4 Click  **Study**.
- 5 In the **Select Study** tree, select **General Studies > Time Dependent**.
- 6 Click  **Done**.

GLOBAL DEFINITIONS

Load the rate constants from file.

Rate constants

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters I**.
- 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 `pesticide_transport_parameters_1.txt`.




5 In the **Label** text field, type **Rate constants**.

First consider the aldicarb decomposition kinetics in the water pond treated as a perfectly mixed system.

GLOBAL ODES AND DAEs (GE)


Global Equations I (ODEI)

Read in a set of the equations defining the reactions.

- 1 In the **Model Builder** window, under **Component I (comp1) > Global ODEs and DAEs (ge)** click **Global Equations I (ODEI)**.
- 2 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `pesticide_transport_reactions.txt`.
- 5 Locate the **Units** section. Click  **Select Dependent Variable Quantity**.
- 6 In the **Physical Quantity** dialog, type **concentration** in the text field.
- 7 In the tree, select **General > Concentration (mol/m³)**.
- 8 Click **OK**.
- 9 In the **Settings** window for **Global Equations**, locate the **Units** section.
- 10 Click  **Select Source Term Quantity**.
- 11 In the **Physical Quantity** dialog, type **reactionrate** in the text field.
- 12 In the tree, select **Transport > Reaction rate (mol/(m³*s))**.
- 13 Click **OK**.

STUDY I

Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Study I** 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, 1, 100).
- 5 In the **Study** toolbar, click  **Compute**.

RESULTS

Concentration of species (100 days)

A plot showing the time dependent concentration is added automatically. Edit this plot to reproduce [Figure 3](#) with the following steps:

- 1 In the **Settings** window for **ID Plot Group**, type Concentration of species (100 days) in the **Label** text field.
- 2 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 3 Locate the **Plot Settings** section.
- 4 Select the **y-axis label** checkbox. In the associated text field, type Concentration (mol/m³).


Global 1

- 1 In the **Model Builder** window, expand the **Concentration of species (100 days)** node, then click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.
- 3 From the **Parameter** list, choose **Expression**.
- 4 In the **Expression** text field, type t.
- 5 From the **Unit** list, choose **d**.

The concentration for all species is added automatically. Add the expression for the sum of the three most toxic species to the table.


- 6 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
cpm_a+cpm_asn+cpm_asx	mol/m ³	Sum of most toxic species

- 7 In the **Concentration of species (100 days)** toolbar, click  **Plot**.


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

ADD PHYSICS



- 1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.
- 3 In the tree, select **Fluid Flow > Porous Media and Subsurface Flow > Richards' Equation (dl)**.
- 4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Study 1**.

- 5 Click the **Add to Component I** button in the window toolbar.
- 6 In the tree, select **Chemical Species Transport > Transport of Diluted Species in Porous Media (tds)**.
- 7 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type 3.
- 8 In the **Concentrations (mol/m³)** table, enter the following settings:

c_a
c_asx
c_asn

- 9 In the table, clear the **Solve** checkbox for **Study 1**.
- 10 Click the **Add to Component I** button in the window toolbar.
- 11 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

ADD STUDY

- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Global ODEs and DAEs (ge)**.
- 4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies > Time Dependent**.
- 5 Click the **Add Study** button in the window toolbar.
- 6 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.



STUDY 2

Step 1: Time Dependent

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

GLOBAL DEFINITIONS

Transport parameters


- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 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 pesticide_transport_parameters_2.txt.
- 5 In the **Label** text field, type Transport parameters.

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 **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** checkbox.
- 7 Clear the **Layers on bottom** checkbox.
- 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.

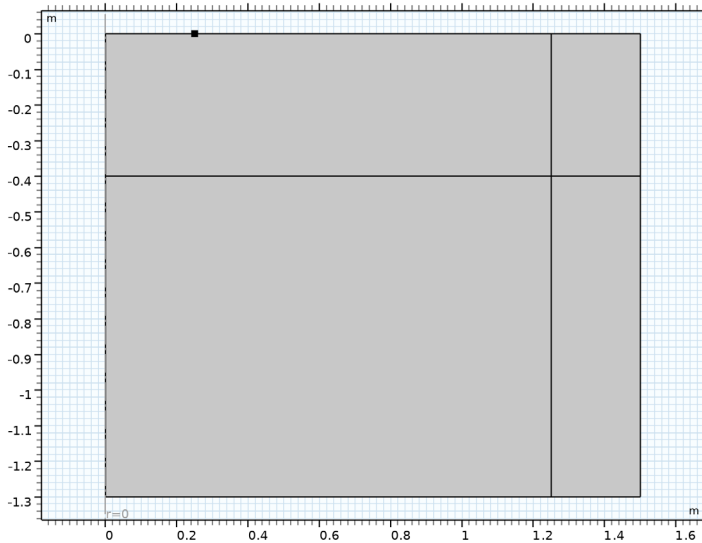
To finish the model geometry, add a point on the top boundary marking the pond's outer rim.

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**.


5 Click the  **Zoom Extents** button in the **Graphics** toolbar.



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**.

Variables 1

1 In the **Definitions** toolbar, click  **Local Variables**.

Load the rate expressions from file.

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

3 Click  **Load from File**.

4 Browse to the model's Application Libraries 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 **Unsaturated Porous Medium** 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)

Unsaturated Porous Medium I

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

- 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 I

- 1 In the **Model Builder** window, click **Liquid I**.
- 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 `d1.theta_1`.
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 (d1)**.
- 7 In the C_m text field, type `d1.Cm`.
- 8 Locate the **Convection** section. From the **u** list, choose **Total Darcy velocity field (d1)**.
The diffusion coefficients are the same for all species.
- 9 Locate the **Diffusion** section. In the $D_{L,ca}$ text field, type `D1`. Also type `D1` in the text fields for the liquid diffusion coefficients of aldicarb sulfoxide and aldicarb sulfone.

Gas I


Again, the diffusion coefficients are the same for all species.

- 1 In the **Model Builder** window, click **Gas I**.
- 2 In the **Settings** window for **Gas**, locate the **Diffusion** section.
- 3 In the $D_{G,ca}$ text field, type `Dg`. Also type `Dg` in the text fields for the gas diffusion coefficients of aldicarb sulfoxide and aldicarb sulfone.
- 4 Locate the **Volatilization** section. In the $k_{G,ca}$ text field, type `kg_a`.
- 5 In the $k_{G,ca,sn}$ text field, type `kg_asn`.

Unsaturated Porous Medium I

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


Adsorption I

- 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_a** checkbox.
- 5 In the $c_{P,ca}$ text field, type kp_a*c_a .
- 6 Select the **Species c_asx** checkbox.
- 7 In the $c_{P,casx}$ text field, type kp_asx*c_asx .
- 8 Select the **Species c_asn** checkbox.
- 9 In the $c_{P,casn}$ text field, type kp_asn*c_asn .

Unsaturated Porous Medium I

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


Dispersion I

- 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 Specify the α matrix as


alphan

alphaz


Reactions I

- 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_{ca} text field, type $d1.\theta_1*(-r_1-r_3)$.
- 5 In the R_{casx} text field, type $d1.\theta_1*(r_1-r_2-r_4)$.
- 6 In the R_{casn} text field, type $d1.\theta_1*(r_2-r_5)$.


Outflow I

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.
- 2 Select Boundaries 2, 8, 12, and 13 only. This corresponds to the right and bottom boundaries.

Concentration I

- 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_a** checkbox.
- 5 In the $c_{0,ca}$ text field, type c0.
- 6 Select the **Species c_asx** checkbox.
- 7 Select the **Species c_asn** checkbox.


Volatilization I

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Volatilization**.
- 2 Select Boundaries 6 and 11 only.
- 3 In the **Settings** window for **Volatilization**, locate the **Volatilization** section.
- 4 In the h_c text field, type Dg/d_s .
- 5 Select the **Species c_a** checkbox.
- 6 Select the **Species c_asn** checkbox.

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/m ³	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/m ³	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**.

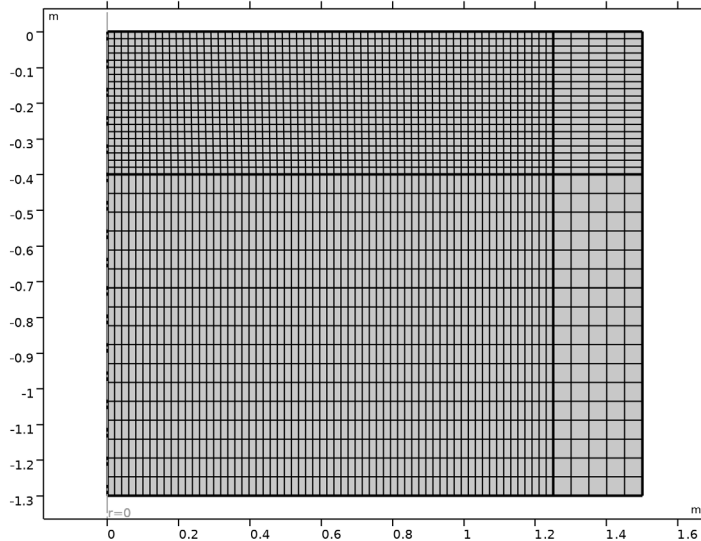
Mapped 1

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.
- 7 Select the **Maximum element size** checkbox. In the associated text field, type 0.02.
- 8 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.





STUDY 2

Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Study 2** 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(1,1,10).
- 5 In the **Model Builder** window, click **Study 2**.
- 6 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 7 Clear the **Generate default plots** checkbox, to disable the automatic generation of default plots. Instead, choose the relevant plots from the Result Templates after computation.
- 8 In the **Study** toolbar, click **Compute**.

RESULT TEMPLATES

First, visualize the pressure head in the revolved geometry. Start with the **Pressure, 3D** result template.

- 1 In the **Results** toolbar, click  **Result Templates** to open the **Result Templates** window.
- 2 Go to the **Result Templates** window.
- 3 In the tree, select **Study 2/Solution 2 (sol2) > Richards' Equation > Pressure, 3D (dl)**.
- 4 Click the **Add Result Template** button in the window toolbar.
- 5 In the **Results** toolbar, click  **Result Templates** to close the **Result Templates** window.


RESULTS

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.

Study 2/Solution 2 (sol2)

In the **Model Builder** window, expand the **Results > Datasets** node, then click **Study 2/Solution 2 (sol2)**.

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.

Pressure Head, 3D (dl)


- 1 In the **Model Builder** window, under **Results** click **Pressure, 3D (dl)**.
- 2 In the **Settings** window for **3D Plot Group**, type Pressure Head, 3D (dl) in the **Label** text field.

Surface

- 1 In the **Model Builder** window, expand the **Pressure Head, 3D (dl)** node, then click **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Viridis**.
- 4 From the **Color table transformation** list, choose **Reverse**.



Contour 1

- 1 In the **Model Builder** window, right-click **Pressure Head, 3D (dl)** 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 8.

- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **GrayScale**.
- 5 Select the **Level labels** checkbox.
- 6 From the **Label color** list, choose **White**.
- 7 Clear the **Color legend** checkbox.
- 8 In the **Pressure Head, 3D (dl)** toolbar, click  **Plot**.

Next, add the result template for the effective saturation.

RESULT TEMPLATES

- 1 In the **Results** toolbar, click  **Result Templates** to open the **Result Templates** window.
- 2 Go to the **Result Templates** window.
- 3 In the tree, select **Study 2/Solution 2 (sol2) > Richards' Equation > Effective Saturation (dl)**.
- 4 Click the **Add Result Template** button in the window toolbar.
- 5 In the **Results** toolbar, click  **Result Templates** to close the **Result Templates** window.

RESULTS

Surface 1

- 1 In the **Model Builder** window, expand the **Effective Saturation (dl)** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table type** list, choose **Discrete**.

Solution Array 1

- 1 Right-click **Surface 1** and choose **Solution Array**. This subnode allows to plot the solution at several output times in one plot group.
- 2 In the **Settings** window for **Solution Array**, locate the **Data** section.
- 3 From the **Time selection** list, choose **From list**.
- 4 In the **Times (d)** list, choose **0.3** and **1**.

Effective Saturation (dl)

- 1 In the **Model Builder** window, under **Results** click **Effective Saturation (dl)**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Color Legend** section.
- 3 From the **Position** list, choose **Bottom**.
- 4 Click to expand the **Plot Array** section. In the **Relative padding** text field, type 0.1.



Arrow Surface 1

- 1 Right-click **Effective Saturation (dl)** and choose **Arrow Surface**.
- 2 In the **Settings** window for **Arrow Surface**, locate the **Coloring and Style** section.
- 3 From the **Color** list, choose **White**.
- 4 Select the **Scale factor** checkbox. In the associated text field, type 20000.
- 5 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Solution Array 1

- 1 Right-click **Arrow Surface 1** and choose **Solution Array**.
- 2 In the **Settings** window for **Solution Array**, locate the **Data** section.
- 3 From the **Time selection** list, choose **From list**.
- 4 In the **Times (d)** list, choose **0.3** and **1**.



Effective Saturation (dl)

- 1 In the **Model Builder** window, under **Results** click **Effective Saturation (dl)**.
- 2 In the **Settings** window for **2D Plot Group**, click to expand the **Title** section.
- 3 From the **Title type** list, choose **None**.
- 4 In the **Effective Saturation (dl)** toolbar, click  **Plot**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Compare the plot in the **Graphics** window with [Figure 5](#).

Continue with adding the plot for the concentration of aldicarb and aldicarb sulfoxide to reproduce [Figure 6](#).

RESULT TEMPLATES

- 1 In the **Results** toolbar, click  **Result Templates** to open the **Result Templates** window.
- 2 Go to the **Result Templates** window.
- 3 In the tree, select **Study 2/Solution 2 (sol2) > Transport of Diluted Species in Porous Media > Concentration, a (tds)**.
- 4 Click the **Add Result Template** button in the window toolbar.
- 5 In the **Results** toolbar, click  **Result Templates** to close the **Result Templates** window.

RESULTS

Comparison of a and asx concentrations

- 1 In the **Model Builder** window, expand the **Results > Concentration, a (tds)** node, then click **Concentration, a (tds)**.

- 2 In the **Settings** window for **2D Plot Group**, type Comparison of a and asx concentrations in the **Label** text field.
- 3 Locate the **Color Legend** section. Select the **Show titles** checkbox.
- 4 Locate the **Plot Array** section. From the **Array type** list, choose **Square**.
- 5 In the **Relative row padding** text field, type 0.1.
- 6 In the **Relative column padding** text field, type 0.2.

Arrow Surface 1

In the **Model Builder** window, right-click **Arrow Surface 1** and choose **Delete**.

Surface 1

- 1 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 2 In the **Color legend title** text field, type a.

Solution Array 1

- 1 Right-click **Surface 1** and choose **Solution Array**.
- 2 In the **Settings** window for **Solution Array**, locate the **Data** section.
- 3 From the **Time selection** list, choose **Manual**.
- 4 In the **Time indices (1-20)** text field, type 19 14 10 to force the images to appear in the right order (earliest output time on the top)
- 5 Locate the **Plot Array** section. From the **Array axis** list, choose **y**.



Surface 1

- 1 In the **Model Builder** window, click **Surface 1**.
- 2 In the **Settings** window for **Surface**, click to expand the **Plot Array** section.
- 3 Select the **Manual indexing** checkbox.

Now set up the concentration plots for aldicarb sulfoxide (asx). You can start from the settings for aldicarb (a).

Surface 2


- 1 Right-click **Results > Comparison of a and asx concentrations > Surface 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type c_asx.
- 4 Locate the **Coloring and Style** section. In the **Color legend title** text field, type asx.
- 5 Locate the **Plot Array** section. In the **Column index** text field, type 1.

- 6 In the **Comparison of a and asx concentrations** toolbar, click  **Plot**.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.



Comparison of a and asx concentrations

- 1 In the **Model Builder** window, click **Comparison of a and asx concentrations**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **None**.

Table Annotation 1

- 1 In the **Comparison of a and asx concentrations** toolbar, click  **More Plots** and choose **Table Annotation**.
- 2 In the **Settings** window for **Table Annotation**, locate the **Data** section.
- 3 From the **Source** list, choose **Local table**.
- 4 In the table, enter the following settings:

x-coordinate	y-coordinate	Annotation
0.2	-1.4	aldicarb (a)
1.45	-1.4	aldicarb sulfoxide (asx)

- 5 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 6 In the **Comparison of a and asx concentrations** toolbar, click  **Plot**.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.