

POLLUTE

Version 8

Example 18: Phase Change



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Version 8

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Description

In this example a phase change in the secondary leachate collection system is modelled using the Phase Change special feature. The landfill has a secondary leachate collection system and liner which overlies a 1 meter thick aquifer. A phase change occurs in the secondary leachate collection system at the interface between the unsaturated and saturated zones, assumed to be .2 and .1 meters thick respectively.

The landfill contains a constant concentration of DCM, which experiences biological decay in the landfill, primary and secondary liners, and the aquifer. A half-life of 10 years in the landfill and 40 years everywhere else is assumed. No biological decay is assumed to occur in the secondary leachate collection system.

The diffusion coefficient of the DCM in the unsaturated zone of the secondary leachate collection system is assumed to be $300 \text{ m}^2/\text{a}$, and in the saturated zone to be $100 \text{ m}^2/\text{a}$ (to represent a high degree of mixing in the saturated zone). The phase change parameter for the DCM in the unsaturated zone is Henry's Constant which is assumed to be 0.1 for DCM in this example.

Two layers are used to model the unsaturated and saturated zones of the .3 meter thick secondary leachate collection system. The first layer represents the unsaturated zone and is .2 meters thick. And the second layer represents the saturated zone and is .1 meter thick.

A Darcy velocity of 0.003 m/a is assumed through the primary liner, and 0 m/a through the secondary liner. Thus, for a 500 meter long landfill the outflow rate in the saturated portion of the secondary leachate collection system would be:

$$\text{Outflow Rate} = (500 * 0.003) / 0.1 = 15 \text{ m/a}$$

This example is for a hypothetical landfill and is used to illustrate how to prepare an input file and run an analysis using the Phase Change option. The example is not a prescription for modeling contaminant migration during operation of a landfill. Each landfill has its own unique characteristics and no general prescription can be made. The Phase Change option should only be used by someone with the hydrogeologic background necessary to appreciate the subtleties associated with the physical situation and the steps necessary for appropriate modeling of this physical situation.

Data Entry

Open the Examples project and open Case 18.

General Tab

Run Auto On Off Save Save As

General Layers Boundaries Special Features Subsurface Model

General Information

Model Title: Case 18: Phase Change

Maximum Depth: 2.65 m

Darcy Velocity: 1 m/year

Laplace Transform Parameters

TAU: 7 N: 20 SIG: 0 RNU: 2

Run Parameters

Output Units

Time Units: yr Depth Units: m Concentration Units: mol/m³

☒ All Depths ☐ Specified Depths

☒ Concentrations at Specified Times ☐ Maximum Concentrations

+ Add X Delete

Time	Units
80	yr
85	yr
90	yr
95	yr
100	yr

The general data for this example is specified on the General tab. The Darcy velocity will be displayed but will be ignored when the Passive Sink option is selected.

Layers Tab

Run Auto On Off Save Save As

General Layers Boundaries Special Features Subsurface Model

+ Add X Delete Copy Paste Move Down Move Up

Name	Sublayers	Thickness	Thickness Units	Dry Density	Density Units	Porosity	Hydrodynamic Dispersion Coefficient	Dispersion Units	Distribution Coefficient	Distribution Units	Fractures	Symbol
Primary Liner	4	0.6	m	1.9	g/cm ³	0.4	0.02	m ² /a	1.5	cm ³ /g	None	
Unsaturated Collection	4	0.2	m	1.9	g/cm ³	0.45	300	m ² /a	0	cm ³ /g	None	
Saturated Collection	4	0.1	m	1.9	g/cm ³	0.45	100	m ² /a	0	cm ³ /g	None	
Secondary Liner	4	0.75	m	1.9	g/cm ³	0.4	0.02	m ² /a	1.5	cm ³ /g	None	

The layer data for this example consists of four layers: a primary liner, a unsaturated collection system, a saturated collection system, and a secondary liner. The data for these layers is specified on the Layers tab.

Boundaries Tab

Run Auto On Off Save Save As

General Layers **Boundaries** Special Features Subsurface Model

Top Boundary

☐ Zero Flux

☒ Constant Concentration

☐ Finite Mass

Concentration 0.04 mol/m³

Bottom Boundary

☐ Zero Flux

☐ Constant Concentration

☒ Fixed Outflow Velocity

☐ Infinite Thickness

Landfill Length: 500 m

Landfill Width: 500 m

Base Thickness: 1 m

Base Porosity: 0.3

Base Outflow Velocity: 3 m/a

Base Symbol

The boundary conditions for this example are a constant concentration top boundary and a fixed outflow bottom boundary. These boundaries can be specified on the Boundaries tab.

Special Features

The biological decay and passive sink data for this model can be entered using the Special Features tab.

Passive Sink

Run Auto On Off Save Save As

General Layers Boundaries **Special Features** Subsurface Model

☐ Initial Concentration Profile
☐ Maximum Sublayer Thickness
☐ Non-linear Sorption
☒ Passive Sink
☐ Print Mass in Base
☒ Radioactive/Biological Decay
☐ Time Varying Properties
☐ Monte Carlo Simulation
☐ Sensitivity Analysis

Passive Sink Radioactive/Biological Decay
 Inflow Rate: ☒ No ☐ Yes Phase Change: ☐ No ☒ Yes
 Interval Type: ☒ Depth Intervals ☐ Layers
 + Add X Delete

Top Depth	Top Depth Units	Bottom Depth	Bottom Depth Units	Darcy Velocity	Darcy Velocity Units	Rate of Removal	Rate of Removal Units	Phase Parameter
0	m	0.6	m	0.003	m/a	0	m/a	1
0.6	m	0.8	m	0.003	m/a	0	m/a	0.1
0.8	m	0.9	m	0.003	m/a	15	m/a	1
0.9	m	1.65	m	0	m/a	0	m/a	1

The passive sink data is used to specify the Phase parameter and the horizontal and vertical Darcy velocities. In this example there are four depth intervals for the passive sink.

Radioactive/Biological Decay

Run Auto On Off Save Save As

General Layers Boundaries **Special Features** Subsurface Model

☐ Initial Concentration Profile
☐ Maximum Sublayer Thickness
☐ Non-linear Sorption
☒ Passive Sink
☐ Print Mass in Base
☒ Radioactive/Biological Decay
☐ Time Varying Properties
☐ Monte Carlo Simulation
☐ Sensitivity Analysis

Passive Sink Radioactive/Biological Decay
 Source Decay: ☒ Yes ☐ No Base Decay: ☒ Yes ☐ No
 Source Half-Life: 10 yr Base Half-Life: 40 yr
 Interval Type: ☒ Depth Intervals ☐ Layers
 + Add X Delete

Top Depth	Top Depth Units	Bottom Depth	Bottom Depth Units	Half-Life	Half-Life Units
0	m	0.6	m	40	yr
0.6	m	0.9	m	0	yr
0.9	m	1.65	m	40	yr

The data for the biological decay of the DCM can be specified by selecting the Radioactive/Biological Decay option on the Special Features tab. In this example there are three decay intervals: one for the primary liner, one for the unsaturated and saturated collection system, and one for the secondary liner.

Model Execution



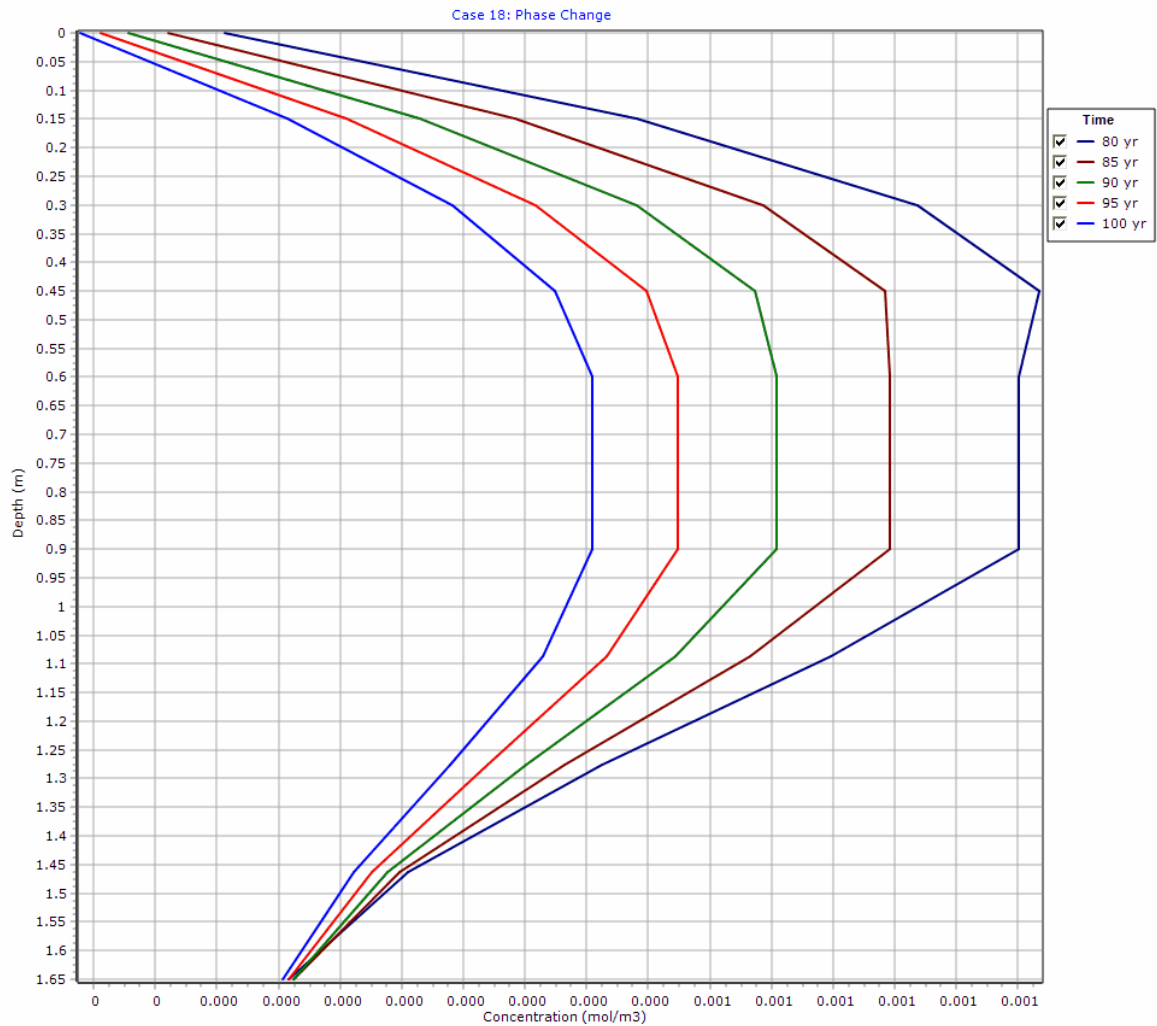
To run the model and calculate the concentrations press the Run button on the toolbar.

Model Output

After the model has been executed, the output for the model will be displayed.

Depth vs Concentration

The Depth vs Concentration chart can be displayed by selecting the Depth vs Concentration item for the Chart Type.



Output Listing

To display the output as a text listing that will show the calculated concentrations as numbers, click on the List tab.

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Case 18: Phase Change

THE PASSIVE SINK OPTION HAS BEEN USED. NOTE THE USER IS RESPONSIBLE FOR ENSURING THAT VELOCITY CHANGES ARE CONSISTENT WITH THE PASSIVE SINK.

Layer Properties

Layer	Thickness	Number of Sublayers	Coefficient of Hydrodynamic Dispersion	Matrix Porosity	Distribution Coefficient	Dry Density
Primary Liner	0.6 m	4	0.02 m ² /a	0.4	1.5 cm ³ /g	1.9 g/cm ³
Unsaturated Collection System	0.2 m	4	300 m ² /a	0.45	0 cm ³ /g	1.9 g/cm ³
Saturated Collection System	0.1 m	4	100 m ² /a	0.45	0 cm ³ /g	1.9 g/cm ³
Secondary Liner	0.75 m	4	0.02 m ² /a	0.4	1.5 cm ³ /g	1.9 g/cm ³

Boundary Conditions

Constant Concentration

Source Concentration = 0.04 mol/m³

Fixed Outflow Bottom Boundary

Landfill Length = 500 m

Landfill Width = 500 m

Base Thickness = 1 m

Base Porosity = 0.3

Base Outflow Velocity = 3 m/a

Radioactive or Biological Decay

Radioactive or Biological Decay Source Half Life = 10 yr

Radioactive or Biological Decay Base Half Life = 40 yr

First Order Radioactive or Biological Decay Depth Ranges

Minimum Depth	Maximum Depth	Half Life
0 m	0.6 m	40 yr
0.6 m	0.9 m	0 yr
0.9 m	1.65 m	40 yr

Velocity and Sink Profile

Time Period	Minimum Depth	Maximum Depth	Vertical Velocity	Horizontal Outflow	Phase Parameter
01	0 m	0.6 m	0.003 m/a	0 m/a	1
	0.6 m	0.8 m	0.003 m/a	0 m/a	0.1
	0.8 m	0.9 m	0.003 m/a	15 m/a	1
	0.9 m	1.65 m	0 m/a	0 m/a	1

Laplace Transform Parameters

TAU = 7 N = 20 SIG = 0 RNU = 2

Calculated Concentrations at Selected Times and Depths

Time yr	Depth m	Concentration mol/m ³
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80	0.000E+00	1.563E-04
	1.500E-01	4.912E-04
	3.000E-01	7.185E-04
	4.500E-01	8.173E-04
	6.000E-01	8.009E-04
	6.500E-01	8.009E-04
	7.000E-01	8.009E-04
	7.500E-01	8.009E-04
	8.000E-01	8.009E-04
	8.250E-01	8.009E-04
	8.500E-01	8.009E-04
	8.750E-01	8.008E-04
	9.000E-01	8.008E-04
	1.088E+00	6.483E-04
	1.275E+00	4.620E-04
	1.463E+00	3.048E-04
	1.650E+00	2.079E-04
85	0.000E+00	1.105E-04
	1.500E-01	3.922E-04
	3.000E-01	5.930E-04
	4.500E-01	6.923E-04
	6.000E-01	6.960E-04
	6.500E-01	6.960E-04
	7.000E-01	6.960E-04
	7.500E-01	6.960E-04
	8.000E-01	6.960E-04
	8.250E-01	6.960E-04
	8.500E-01	6.960E-04
	8.750E-01	6.960E-04
	9.000E-01	6.959E-04
	1.088E+00	5.830E-04
	1.275E+00	4.321E-04
	1.463E+00	2.982E-04
	1.650E+00	2.118E-04
90	0.000E+00	7.816E-05
	1.500E-01	3.151E-04
	3.000E-01	4.912E-04
	4.500E-01	5.870E-04
	6.000E-01	6.040E-04
	6.500E-01	6.040E-04
	7.000E-01	6.040E-04
	7.500E-01	6.040E-04
	8.000E-01	6.040E-04
	8.250E-01	6.040E-04
	8.500E-01	6.040E-04
	8.750E-01	6.040E-04
	9.000E-01	6.040E-04
	1.088E+00	5.220E-04
	1.275E+00	4.010E-04
	1.463E+00	2.881E-04

	1.650E+00	2.118E-04
95	0.000E+00	5.527E-05
	1.500E-01	2.547E-04
	3.000E-01	4.083E-04
	4.500E-01	4.985E-04
	6.000E-01	5.239E-04
	6.500E-01	5.239E-04
	7.000E-01	5.239E-04
	7.500E-01	5.239E-04
	8.000E-01	5.239E-04
	8.250E-01	5.239E-04
	8.500E-01	5.239E-04
	8.750E-01	5.239E-04
	9.000E-01	5.239E-04
	1.088E+00	4.659E-04
	1.275E+00	3.698E-04
	1.463E+00	2.754E-04
	1.650E+00	2.087E-04
100	0.000E+00	3.908E-05
	1.500E-01	2.072E-04
	3.000E-01	3.408E-04
	4.500E-01	4.242E-04
	6.000E-01	4.544E-04
	6.500E-01	4.544E-04
	7.000E-01	4.544E-04
	7.500E-01	4.544E-04
	8.000E-01	4.544E-04
	8.250E-01	4.544E-04
	8.500E-01	4.544E-04
	8.750E-01	4.544E-04
	9.000E-01	4.544E-04
	1.088E+00	4.149E-04
	1.275E+00	3.392E-04
	1.463E+00	2.609E-04
	1.650E+00	2.029E-04

NOTICE

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