

POLLUTE

Version 8

Example 8: Diffusion with Initial Concentration Profile



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Description

The results of a laboratory diffusion test are analyzed in this example [see Rowe, Caers & Barone, 1988; Barone, Yanful, Quigley & Rowe, 1989]. In this example the diffusion of Potassium in a clay is examined. The clay has an initial background concentration of Potassium of 10 mg/L.

The leachate source has an initial concentration (c_o) of 400 mg/L, and the physical height of the leachate in the reservoir above the soil was 6 cm. At the base of the specimen there was an impermeable barrier (i.e., zero flux).

Following are the parameters used in this example:

Property	Symbol	Value	Units
Darcy Velocity	v_a	0	m/a
Diffusion Coefficient	D	0.648	cm ² /d
Distribution Coefficient	K_d	2.68	cm ³ /g
Soil Porosity	n_m	0.39	-
Dry Density		1.68	g/cm ³
Soil Layer Thickness	H	4.5	cm
Number of Sub-layers		10	-
Source Concentration	c_o	400	mg/L
Ref. Height of Leachate	H_r	6	cm
Background Concentration		10	mg/L

When using an initial concentration profile (eg. background 10 mg/L in this example) the user should have at least three layers, with the top and bottom layer being very thin. In this example layers 1 and 3 are taken to be 0.1 cm thick and layer 2 (the main layer) is taken to be 4.5 - 0.2 = 4.3 cm thick.

Data Entry

Open the Examples project and open Case 8.

General Tab

The screenshot shows the software interface with the following settings:

- General Information:** Model Title: Case 8: Diffusion with initial concentration profile; Maximum Depth: 4.5 cm; Darcy Velocity: 0 m/year.
- Laplace Transform Parameters:** TAU: 7; N: 20; SIG: 0; RNU: 2.
- Run Parameters:** Output Units: Time Units: day; Depth Units: cm; Concentration Units: mg/L.
- Concentration Calculation:** Concentrations at Specified Times (selected).
- Specified Times Table:**

Time	Units
3	day
6	day
9	day
12	day
15	day

On the General tab the Darcy velocity is set to zero for pure diffusion. The concentrations can either be calculated at specified times or the time of the maximum concentration can be found. In this example the concentrations will be calculated at 5 times: 3, 6, 9, 12, and 15 years.

Layers Tab

Name	Sublayers	Thickness	Thickness Units	Dry Density	Density Units	Porosity	Hydrodynamic Dispersion Coefficient	Dispersion Units	Distribution Coefficient	Distribution Units	Fractures	Symbol
Clay	1	0.1	cm	1.68	g/cm ³	0.39	0.648	cm ² /day	2.68	cm ³ /g	None	▨
Clay	10	4.3	cm	1.68	g/cm ³	0.39	0.648	cm ² /day	2.68	cm ³ /g	None	▨
Clay	1	0.1	cm	1.68	g/cm ³	0.39	0.648	cm ² /day	2.68	cm ³ /g	None	▨

There are no fractures in these layers. For pure diffusion even if there were fractures it should be modelled as if the soil was unfractured, since there would be no flow in the fractures for pure diffusion.

Boundaries Tab

The screenshot shows the 'Boundaries' tab in the software. The 'Top Boundary' section has three radio buttons: 'Zero Flux' (unselected), 'Constant Concentration' (unselected), and 'Finite Mass' (selected). Below these are three input fields: 'Initial Source Concentration' (400 mg/L), 'Rate of Concentration Increase' (0 mg/L/yr), and 'Volume of Leachate Collected' (0 m/a). A 'Specify' section has two radio buttons: 'Reference Height of Leachate' (selected) and 'Waste Properties' (unselected). Below that is a 'Reference Height of Leachate' input field (6 cm). The 'Bottom Boundary' section has four radio buttons: 'Zero Flux' (selected), 'Constant Concentration' (unselected), 'Fixed Outflow Velocity' (unselected), and 'Infinite Thickness' (unselected).

In this example, the top boundary has a finite mass and the bottom boundary is represented as a zero flux layer.

Special Features

The initial concentration profile for this example is specified using the Special Features tab.

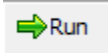
Initial Concentration Profile

The screenshot shows the 'Special Features' tab in the software. The 'Initial Concentration Profile' checkbox is checked. Other checkboxes include 'Maximum Sublayer Thickness', 'Non-linear Sorption', 'Passive Sink', 'Print Mass in Base', 'Radioactive/Biological Decay', 'Time Varying Properties', 'Monte Carlo Simulation', and 'Sensitivity Analysis'. The 'Initial Concentration Profile' section has three input fields: 'Start Time' (0 yr), 'Flux into Soil' (0 m²/a), and 'Flux into Base' (0 m²/a). The 'Interval Type' section has two radio buttons: 'Depth Intervals' (selected) and 'Sublayers' (unselected). Below this is a table with columns: 'Top Depth', 'Top Depth Units', 'Bottom Depth', 'Bottom Depth Units', 'Concentration', and 'Concentration Units'. The table contains one row with values: 0, cm, 4.5, cm, 10, mg/L.

Top Depth	Top Depth Units	Bottom Depth	Bottom Depth Units	Concentration	Concentration Units
0	cm	4.5	cm	10	mg/L

To specify the initial concentration profile, check the Initial Concentration Profile box on the Special Features tab.

Model Execution



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

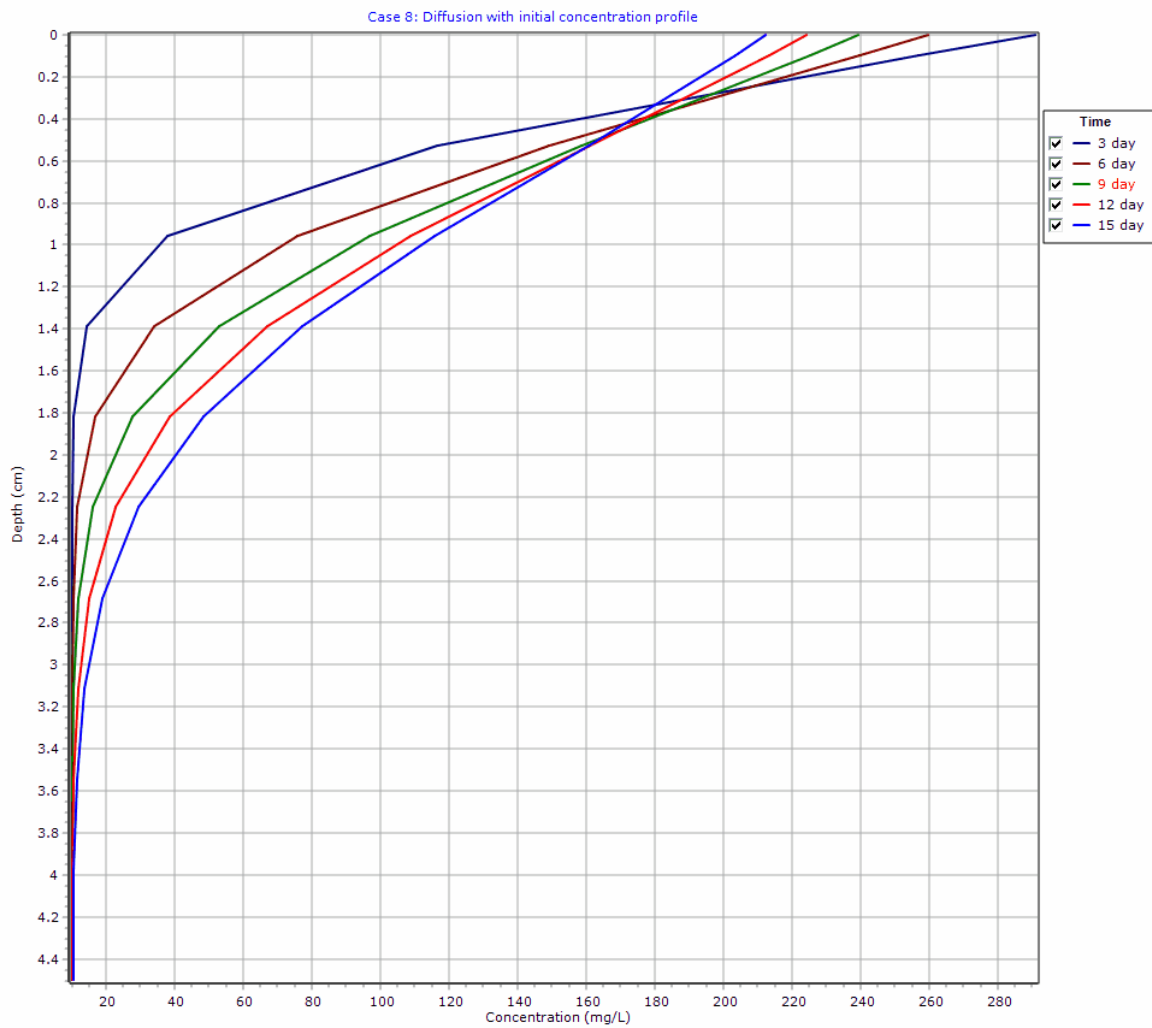
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Model Output

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 8: Diffusion with initial concentration profile

THE DARCY VELOCITY (Flux) THROUGH THE LAYERS $V_a = 0$ m/year

Layer Properties

Layer	Thickness	Number of Sublayers	Coefficient of Hydrodynamic Dispersion	Matrix Porosity	Distribution Coefficient	Dry Density
Clay	0.1 cm	1	0.648 cm ² /day	0.39	2.68 cm ³ /g	1.68 g/cm ³
Clay	4.3 cm	10	0.648 cm ² /day	0.39	2.68 cm ³ /g	1.68 g/cm ³
Clay	0.1 cm	1	0.648 cm ² /day	0.39	2.68 cm ³ /g	1.68 g/cm ³

Boundary Conditions**Finite Mass Top Boundary**

Initial Concentration = 400 mg/L
 Rate of Increase = 0 mg/L/yr
 Volume of Leachate Collected = 0 m³/a
 Thickness of Waste = 0 m
 Waste Density = 0 kg/m³
 Proportion of Mass = 0
 Volumetric Water Content = 0
 Conversion Rate Half Life = 0 year
 Reference Height of Leachate = 6 cm

Zero Flux Bottom Boundary**INITIAL CONCENTRATION PROFILE**

Time = 0 yr
 Flux into Soil = 0 m²/a
 Flux into Base = 0 m²/a

Top Depth	Bottom Depth	Concentration
0 cm	4.5 cm	10 mg/L

Laplace Transform Parameters

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

Calculated Concentrations at Selected Times and Depths

Time day	Depth cm	Concentration mg/L
3	0.000E+00	2.910E+02
	1.000E-01	2.569E+02
	5.300E-01	1.164E+02
	9.600E-01	3.779E+01
	1.390E+00	1.426E+01
	1.820E+00	1.038E+01
	2.250E+00	1.002E+01
	2.680E+00	1.000E+01
	3.110E+00	1.000E+01
	3.540E+00	1.000E+01
3.970E+00	1.000E+01	

	4.400E+00	1.000E+01
	4.500E+00	1.000E+01
6	0.000E+00	2.596E+02
	1.000E-01	2.398E+02
	5.300E-01	1.491E+02
	9.600E-01	7.573E+01
	1.390E+00	3.391E+01
	1.820E+00	1.664E+01
	2.250E+00	1.140E+01
	2.680E+00	1.022E+01
	3.110E+00	1.003E+01
	3.540E+00	1.000E+01
	3.970E+00	1.000E+01
	4.400E+00	1.000E+01
	4.500E+00	1.000E+01
9	0.000E+00	2.394E+02
	1.000E-01	2.253E+02
	5.300E-01	1.586E+02
	9.600E-01	9.690E+01
	1.390E+00	5.273E+01
	1.820E+00	2.758E+01
	2.250E+00	1.602E+01
	2.680E+00	1.172E+01
	3.110E+00	1.040E+01
	3.540E+00	1.008E+01
	3.970E+00	1.001E+01
	4.400E+00	1.000E+01
	4.500E+00	1.000E+01
12	0.000E+00	2.243E+02
	1.000E-01	2.135E+02
	5.300E-01	1.610E+02
	9.600E-01	1.088E+02
	1.390E+00	6.682E+01
	1.820E+00	3.859E+01
	2.250E+00	2.256E+01
	2.680E+00	1.480E+01
	3.110E+00	1.160E+01
	3.540E+00	1.046E+01
	3.970E+00	1.012E+01
	4.400E+00	1.004E+01
	4.500E+00	1.003E+01
15	0.000E+00	2.124E+02
	1.000E-01	2.036E+02
	5.300E-01	1.605E+02
	9.600E-01	1.158E+02
	1.390E+00	7.699E+01
	1.820E+00	4.814E+01
	2.250E+00	2.948E+01
	2.680E+00	1.891E+01
	3.110E+00	1.365E+01

	3.540E+00	1.134E+01
	3.970E+00	1.045E+01
	4.400E+00	1.020E+01
	4.500E+00	1.019E+01

NOTICE

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