POLLUTE

Version 8

Example 8: Diffusion with Initial Concentration Profile

GAEA Technologies Ltd,

221 Laurel Street
Cambridge, Ontario
Canada
N3H 3Y6

Tel: (613) 900-1950

Email:
sales@gaeatech.com
support@gaeatech.com

www.gaeatech.com

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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:

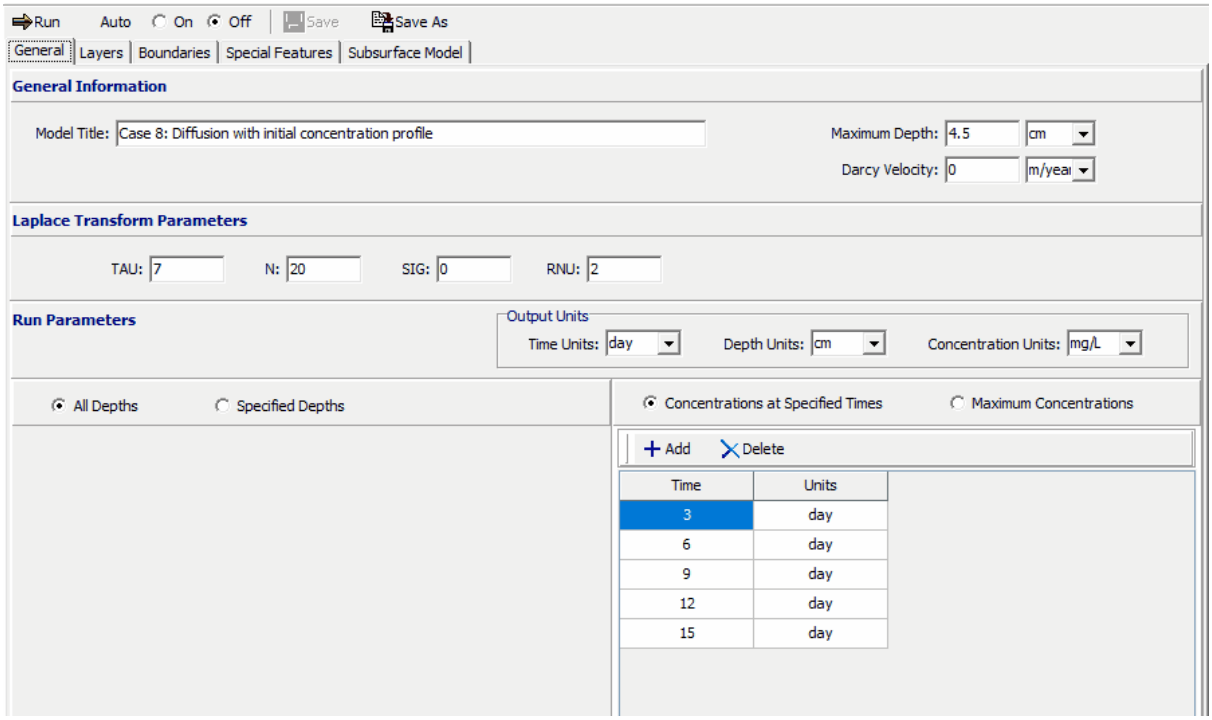
Property	Symbol	Value	Units
Darcy Velocity	v_a	0	m/a
Diffusion Coefficient	D	0.648	cm^2/d
Distribution Coefficient	K_d	2.68	cm^3/g
Soil Porosity	n_m	0.39	-
Dry Density		1.68	g/cm^3
Soil Layer Thickness	H	4.5	cm
Number of Sub-layers		10	-
Source Concentration	c_o	400	mg/L
Ref. Height of Leachate	H_r	6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

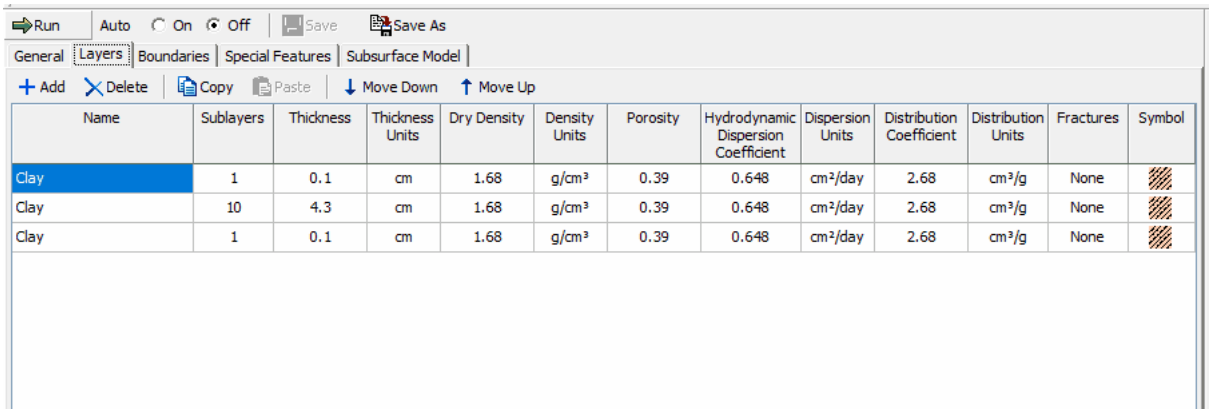
Open the Examples project and open Case 8.

General Tab



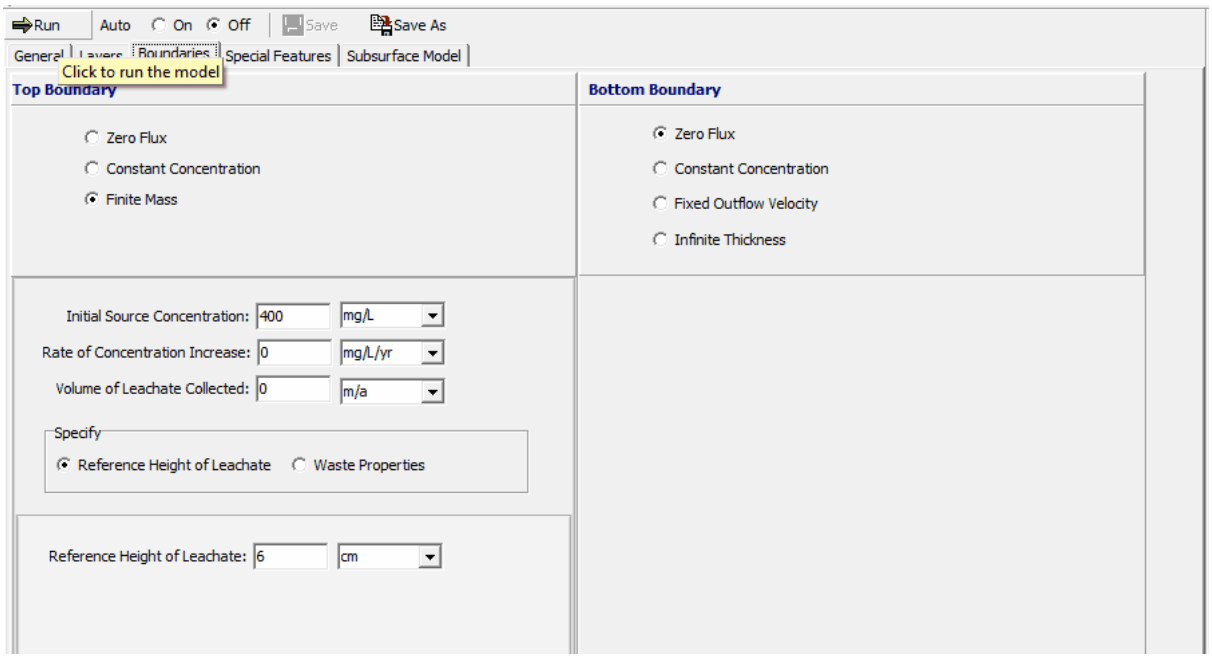
On the General tab the Darcy velocity is set to zero for pure diffusion. The concentrations can either be calculated at specified times or the time of the maximum concentration can be found. In this example the concentrations will be calculated at 5 times: 3, 6, 9,
12, and 15 years.

Layers Tab



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

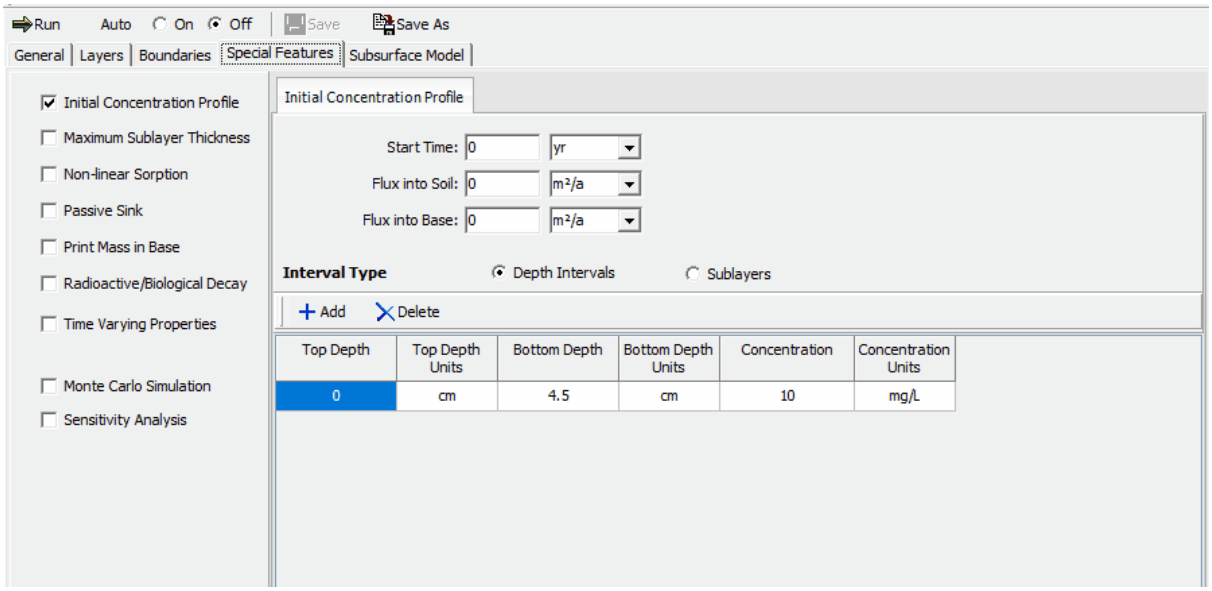


In this example, the top boundary has a finite mass and the bottom boundary is represented as a zero flux layer.

Special Features

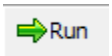
The initial concentration profile for this example is specified using the Special Features tab.

Initial Concentration Profile



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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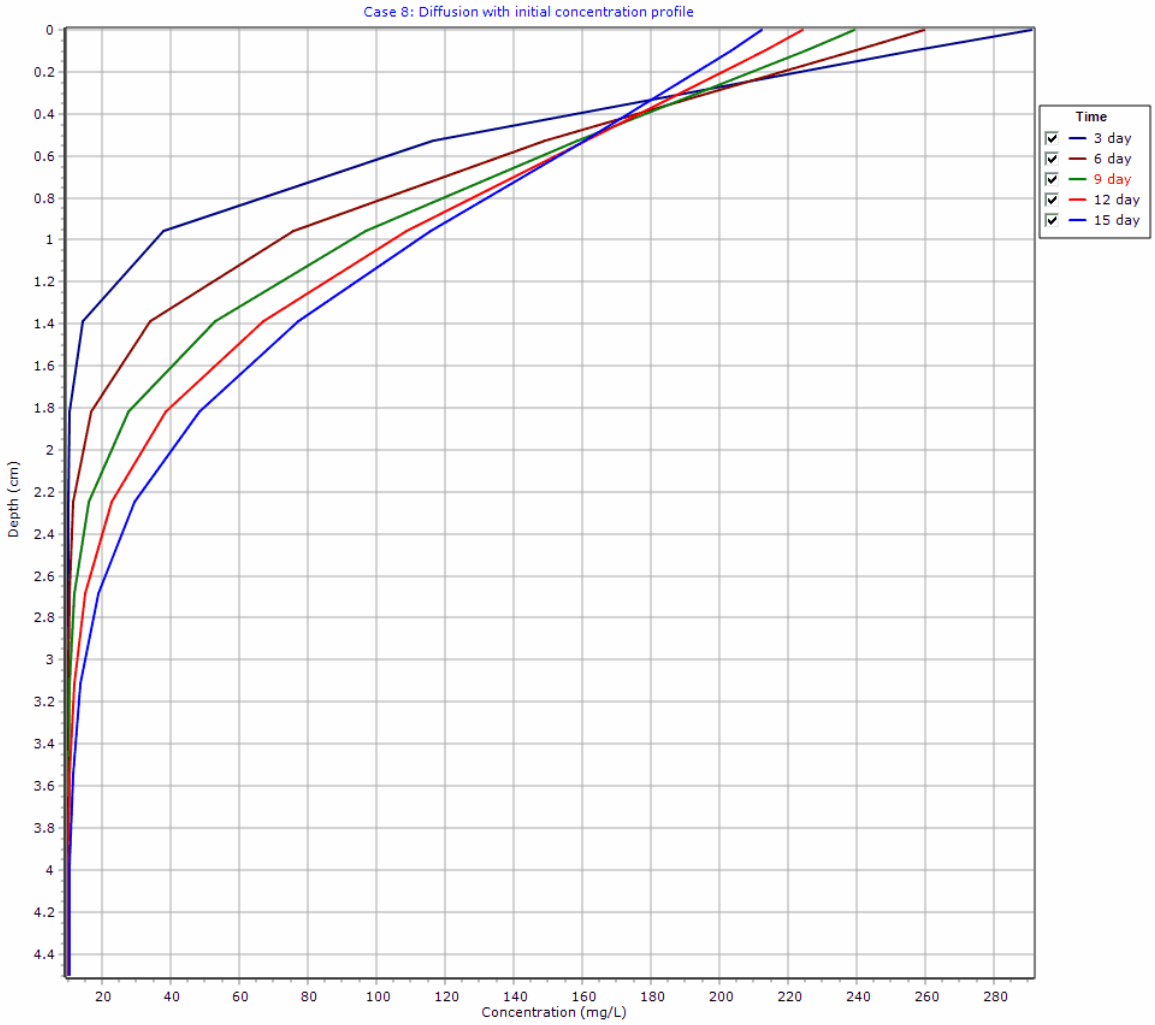
Model Output

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 Va = 0 m/year

Layer Properties

Layer	Thickness	Number of Sublayers	Coefficient of Hydrodynamic Dispersion	Matrix Porosity	Distributon Coefficient	Dry Density
Clay	0.1 cm	1	0.648 cm²/day	0.39	2.68 cm³/g	1.68 g/cm³
Clay	4.3 cm	10	0.648 cm²/day	0.39	2.68 cm³/g	1.68 g/cm³
Clay	0.1 cm	1	0.648 cm²/day	0.39	2.68 cm³/g	1.68 g/cm³

Boundary Conditions

Finite Mass Top Boundary

Initial Concentration = 400 mg/L
Rate of Increase = 0 mg/L/yr
Volume of Leachate Collected = 0 m/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