POLLUTE

Version 8

Example 9: Freundlich Non-linear Sorption

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

In this example a laboratory test is simulated using diffusion and Freundlich non-linear sorption. The sample is a 7 cm thick clay with an impermeable base and a finite mass source of Phenol. The leachate source has an initial concentration (c_o) of 50 mg/L, and the physical height of the leachate in the reservoir above the soil was 6.5 cm. Parameters for the Freundlich isotherm were obtained experimentally from batch tests, these are K_f=2 and =0.628.

Following are the parameters used in this example:

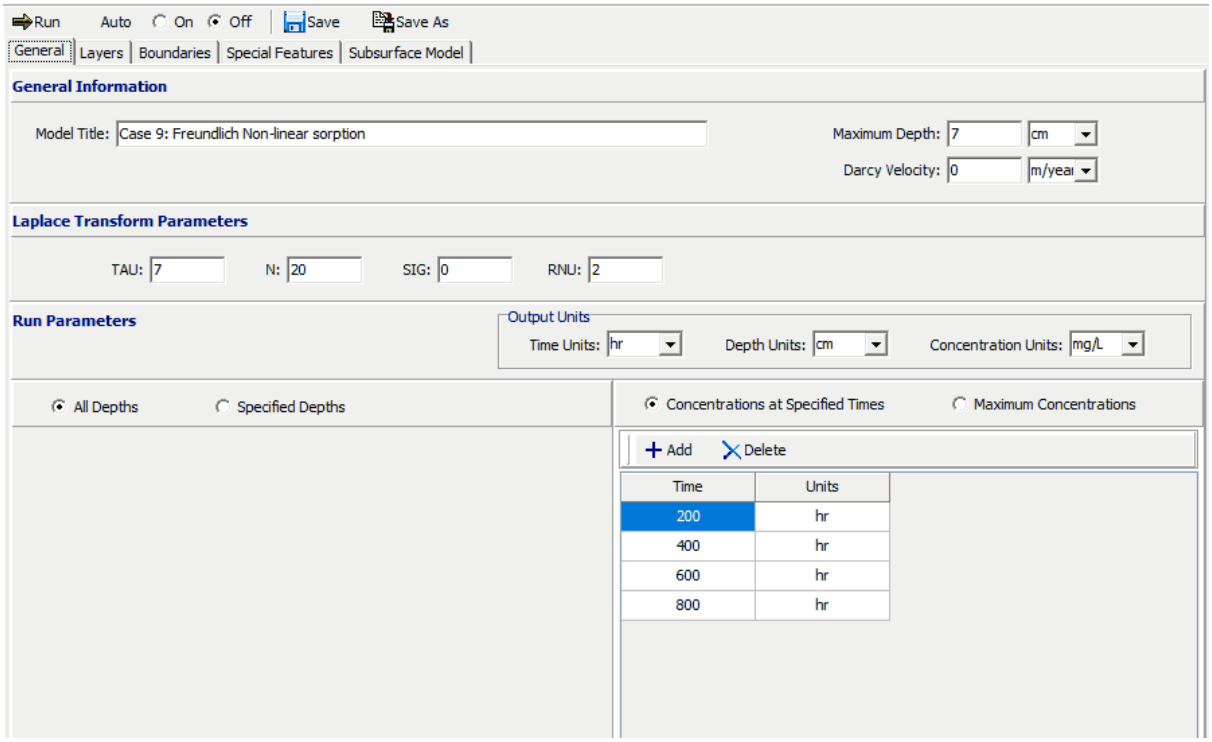
Property	Symbol	Value	Units
Darcy Velocity	v_a	0	m/a
Diffusion Coefficient	D	0.019	cm^2/hr
Sorption Coefficient	K_f	2	cm^3/g
Soil Porosity	n	0.46	-
Dry Density		1.47	g/cm^3
Soil Layer Thickness	H	7	cm
Number of Sub-layers		14	-
Source Concentration	c_o	50	mg/L
Ref. Height of Leachate	H_r	6.5	cm

When using non-linear sorption the accuracy of the solution is dependent on the number of sub-layers used.

Data Entry

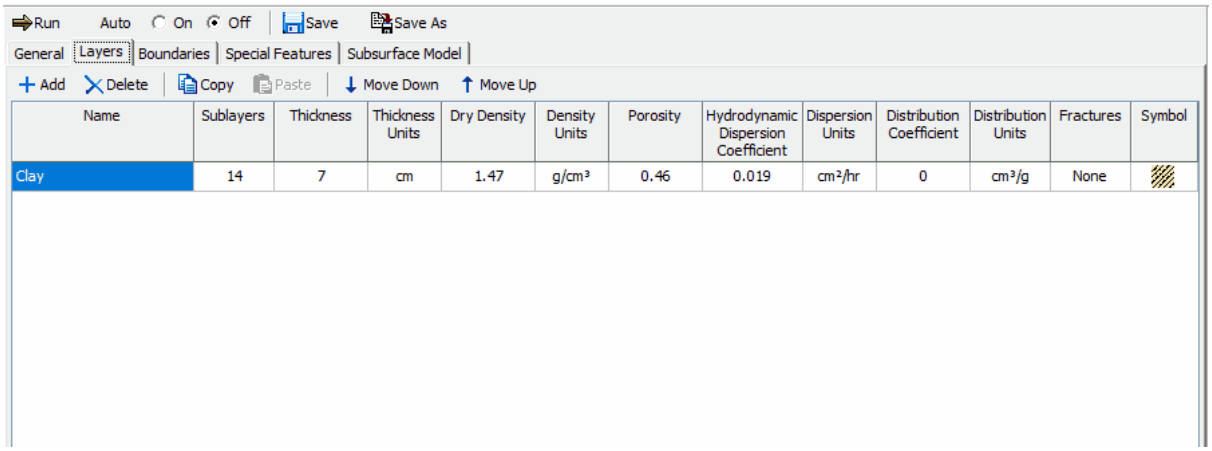
Open the Examples project and open Case 9.

General Tab



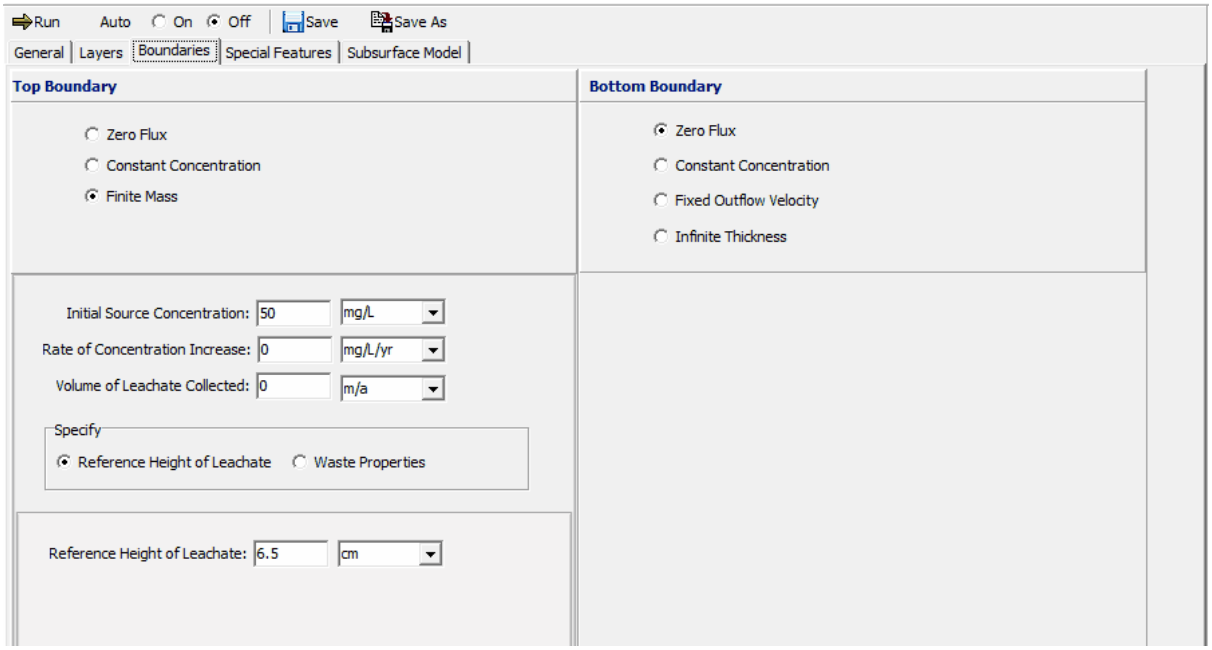
On the General tab the Darcy velocity is set to zero for pure diffusion. The concentrations can either be calculated at specified times or the time of the maximum concentration can be found. In this example the concentrations will be calculated at 4 times: 200, 400, 600, and 800 years.

Layers Tab



When using non-linear sorption the Distribution Coefficient is automatically calculated. The value entered on this tab is ignored by the program.There are no fractures in the layer. 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 through the matrix.

Boundaries Tab

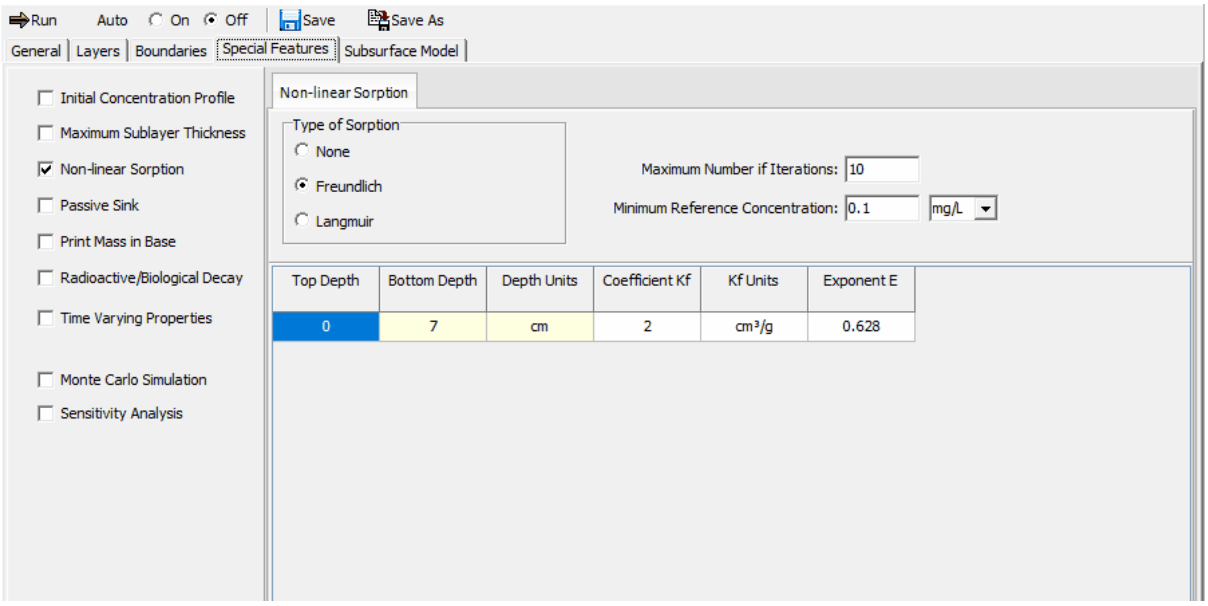


In this example, the top boundary has a finite mass and the bottom boundary is represented as a zero flux layer.

Special Features

The non-linear sorption for this example is specified using the Special Features tab.

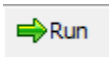
Non-linear Sorption



To specify the Freundlich non-linear sorption, check the Non-linear Sorption box on the Special Features tab. The Non-linear Sorption Data sub-tab can be used to specify the type of sorption as either Freundlich or Langmuir.

The Freundlich non-linear sorption parameters are determined experimentally. The iterative procedure used to determine the distribution coefficient is repeated until either the maximum change in concentrations between iterations is less than 0.1% or the
maximum number of iterations is reached. Minimum reference concentration is the minimum value that will be used in calculating the distribution coefficient. If the average concentration in a sub-layer is less than this minimum reference value, then the reference value is used in the calculation of the distribution coefficient.

Model Execution



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

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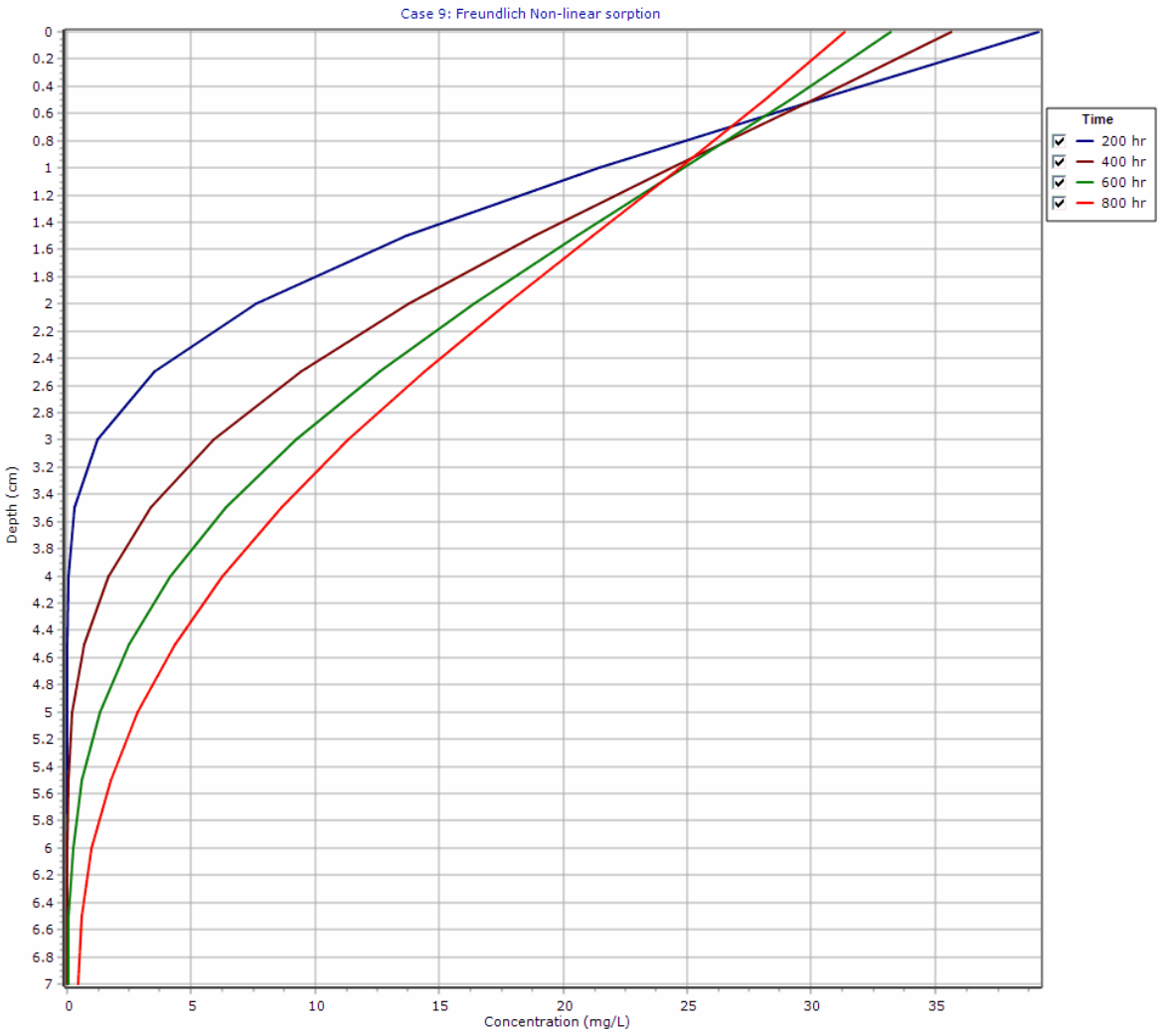
Model Output

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 9: Freundlich Non-linear sorption

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	7 cm	14	0.019 cm²/hr	0.46	0 cm³/g	1.47 g/cm³

Non-Linear Sorption

Maximum Number of Iterations = 10
Minimum Reference Concentration = 0.1 mg/L

Freundlich Sorption Isotherm S = Kf * c^E

Layer	Kf	E
Clay	2	0.628

Boundary Conditions

Finite Mass Top Boundary

Initial Concentration = 50 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 = 6.5 cm

Zero Flux Bottom Boundary

Laplace Transform Parameters

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

Calculated Concentrations at Selected Times and Depths

Time hr	Depth cm	Concentration mg/L
200	0.000E+00	3.915E+01
	5.000E-01	3.022E+01
	1.000E+00	2.143E+01
	1.500E+00	1.367E+01
	2.000E+00	7.618E+00
	2.500E+00	3.521E+00
	3.000E+00	1.233E+00
	3.500E+00	2.728E-01
	4.000E+00	3.002E-02
	4.500E+00	1.801E-03
	5.000E+00	6.511E-05
	5.500E+00	1.412E-06
	6.000E+00	1.834E-08

	6.500E+00	1.499E-10
	7.000E+00	5.539E-12
400	0.000E+00	3.562E+01
	5.000E-01	3.009E+01
	1.000E+00	2.439E+01
	1.500E+00	1.884E+01
	2.000E+00	1.376E+01
	2.500E+00	9.404E+00
	3.000E+00	5.917E+00
	3.500E+00	3.349E+00
	4.000E+00	1.645E+00
	4.500E+00	6.591E-01
	5.000E+00	1.935E-01
	5.500E+00	3.828E-02
	6.000E+00	5.748E-03
	6.500E+00	6.747E-04
	7.000E+00	1.213E-04
600	0.000E+00	3.321E+01
	5.000E-01	2.914E+01
	1.000E+00	2.486E+01
	1.500E+00	2.057E+01
	2.000E+00	1.643E+01
	2.500E+00	1.261E+01
	3.000E+00	9.239E+00
	3.500E+00	6.408E+00
	4.000E+00	4.156E+00
	4.500E+00	2.478E+00
	5.000E+00	1.324E+00
	5.500E+00	6.085E-01
	6.000E+00	2.267E-01
	6.500E+00	6.795E-02
	7.000E+00	3.012E-02
800	0.000E+00	3.136E+01
	5.000E-01	2.812E+01
	1.000E+00	2.469E+01
	1.500E+00	2.119E+01
	2.000E+00	1.772E+01
	2.500E+00	1.441E+01
	3.000E+00	1.135E+01
	3.500E+00	8.617E+00
	4.000E+00	6.273E+00
	4.500E+00	4.347E+00
	5.000E+00	2.841E+00
	5.500E+00	1.736E+00
	6.000E+00	9.974E-01
	6.500E+00	5.794E-01
	7.000E+00	4.451E-01

Convergence Check for Non-linear Sorption

Time	Iterations	Maximum Change

hr		
200	10	0.162
400	9	0.0977
600	9	0.0325
800	8	0.0783

NOTICE

Although this program has been tested and experience would indicate that it is accurate within the limits given by the assumptions of the theory used, we make no warranty as to workability of this software or any other licensed material. No warranties either expressed or implied (including warranties of fitness) shall apply. No responsibility is assumed for any errors, mistakes or misrepresentations that may occur from the use of this computer program. The user accepts full responsibility for assessing the validity and applicability of the results obtained with this program for any specific case.