

POLLUTE

Version 8

Example 9: Freundlich Non-linear Sorption



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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 $n=0.628$.

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

Run Auto On Off Save Save As

General Layers Boundaries Special Features Subsurface Model

General Information

Model Title: Case 9: Freundlich Non-linear sorption

Maximum Depth: 7 cm

Darcy Velocity: 0 m/year

Laplace Transform Parameters

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

Run Parameters

Output Units

Time Units: hr Depth Units: cm Concentration Units: mg/L

☒ All Depths ☐ Specified Depths

☒ Concentrations at Specified Times ☐ Maximum Concentrations

+ Add X Delete

Time	Units
200	hr
400	hr
600	hr
800	hr

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

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
Clay	14	7	cm	1.47	g/cm ³	0.46	0.019	cm ² /hr	0	cm ³ /g	None	

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

Top Boundary

☐ Zero Flux
☐ Constant Concentration
☒ Finite Mass

Initial Source Concentration: 50 mg/L
 Rate of Concentration Increase: 0 mg/L/yr
 Volume of Leachate Collected: 0 m/a

Specify

☒ Reference Height of Leachate ☐ Waste Properties

Reference Height of Leachate: 6.5 cm

Bottom Boundary

☒ Zero Flux
☐ Constant Concentration
☐ Fixed Outflow Velocity
☐ Infinite Thickness

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

☐ 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

Non-linear Sorption

Type of Sorption:
☐ None
☒ Freundlich
☐ Langmuir

Maximum Number of Iterations: 10

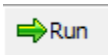
Minimum Reference Concentration: 0.1 mg/L

Top Depth	Bottom Depth	Depth Units	Coefficient Kf	Kf Units	Exponent E
0	7	cm	2	cm ³ /g	0.628

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.

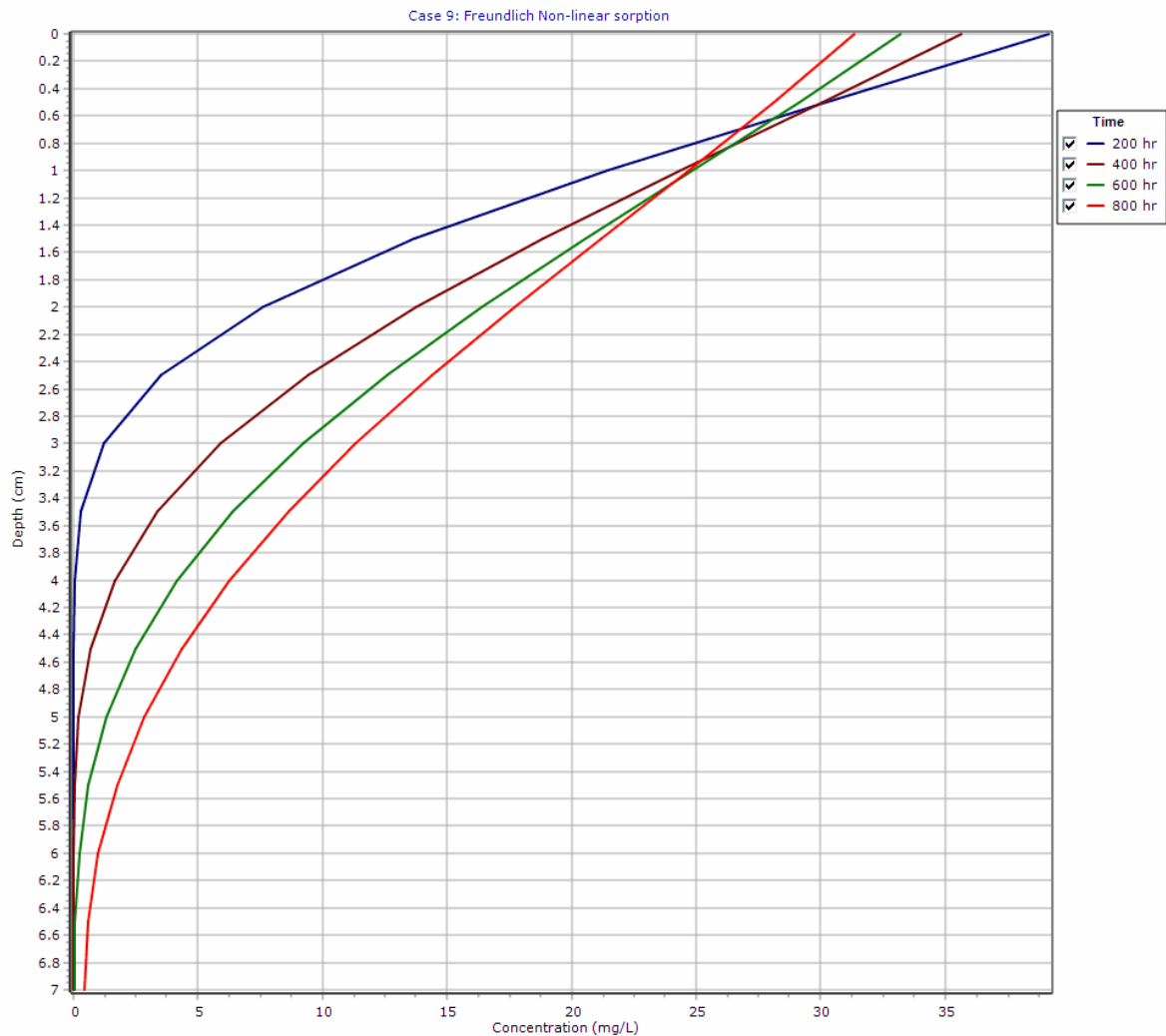
.

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 $V_a = 0$ m/year

Layer Properties

Layer	Thickness	Number of Sublayers	Coefficient of Hydrodynamic Dispersion	Matrix Porosity	Distribution Coefficient	Dry Density
Clay	7 cm	14	0.019 cm ² /hr	0.46	0 cm ³ /g	1.47 g/cm ³

Non-Linear Sorption

Maximum Number of Iterations = 10

Minimum Reference Concentration = 0.1 mg/L

Freundlich Sorption Isotherm $S = K_f * c^E$

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

NOTICE

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