

POLLUTE

Version 8

Example 7: Fractured Rock and Radioactive Decay



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Description

This example illustrates the use of the program for lateral migration of a radioactive contaminant in a fractured porous rock with a single set of parallel fractures. It considers advective-dispersive transport along the fractures and diffusion into the rock matrix. The deposit is assumed to extend a considerable distance from the source (effectively an infinite distance) but we are only interested here in what happens over the first 50 m after 30 years..

It is assumed that the source concentration, c_o , is 1 unit and that the half life of the radioactive species is 100 years. The source is considered to have a sufficiently large supply that there is no significant change in source concentration due to mass movement into the rock. However the source does experience radioactive decay.

This example is also being used to illustrate the Maximum Sublayer Thickness Special Feature, for specifying sublayer thicknesses that are greater than 5 units.

The following parameters are defined for this example:

Property	Symbol	Value	Units
Darcy Velocity	v_a	0.08	m/a
Fractured Rock Thickness	H_T	50	m
Number of Sub-layers		5	-
Fracture spacing	$2H_1$	0.05	m
Fracture opening	$2h_1$	10	μm
Dispersion along fractures	D_f	6	m^2/a
Fracture Distribution Coefficient	K_f	0	cm^3/g
Matrix Diffusion Coefficient	D_m	0.0018	m^2/a
Matrix Distribution Coefficient	K_m	0	cm^3/g
Matrix Porosity	n_m	0.05	-
Dry Density of Matrix		2	g/cm^3
Source Concentration	c_o	1	
Half life of contaminant		100	a
Time period of interest		30	a

Data Entry

Open the Examples project and open Case 7.

General Tab

The screenshot shows the software interface with the following settings:

- General Information:** Model Title: "Case 7: Fractured rock and radioactive decay", Maximum Depth: 50 m, Darcy Velocity: 0.08 m/year.
- Laplace Transform Parameters:** TAU: 7, N: 40, SIG: 0, RNU: 4.
- Run Parameters:** Output Units: Time Units: year, Depth Units: m, Concentration Units: mg/L.
- Depth Selection:** Radio button "Specified Depths" is selected. A table lists depths: 10 m, 30 m, 40 m, and 50 m.
- Time Selection:** Radio button "Concentrations at Specified Times" is selected. A table lists a time of 30 years.

On the General tab the integration parameters for the Laplace Transform have been increased for this example. These parameters will need to be adjusted if the output shows that the default parameters are insufficient.

The times and depths to calculate the concentrations is set in the Run Parameters at the bottom of the tab. 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 a time of 30 years and at 4 depths: 10, 30, 40, and 50 m.

Layers Tab

The screenshot shows the Layers Tab with the following data:

Name	Sublayers	Thickness	Thickness Units	Dry Density	Density Units	Porosity	Hydrodynamic Dispersion Coefficient	Dispersion Units	Distribution Coefficient	Distribution Units	Fractures	Symbol
Fractured Rock	5	50	m	2	g/cm ³	0.05	0.0018	m ² /a	0	m ³ /kg	1	

On this tab the data for the layer and fracture can be added.

Boundaries Tab

The screenshot shows the 'Boundaries' tab in a software application. The interface is divided into two main sections: 'Top Boundary' and 'Bottom Boundary'.
 In the 'Top Boundary' section, three radio button options are present: 'Zero Flux', 'Constant Concentration' (which is selected), and 'Finite Mass'. Below these options, there is a text input field containing the number '1' and a dropdown menu set to 'mg/L'.
 In the 'Bottom Boundary' section, four radio button options are present: 'Zero Flux', 'Constant Concentration', 'Fixed Outflow Velocity', and 'Infinite Thickness' (which is selected). To the right of these options, there is a 'Base Symbol' button and a small square icon with a green and yellow grid pattern.

In this example, the top boundary has a constant concentration and the bottom boundary is represented as a layer with infinite thickness. For the Infinite Thickness boundary condition, the properties of the last layer in the Layer Data are assumed to extend infinitely.

Special Features

The radioactive decay and maximum sublayer thickness for this example are specified using the Special Features tab.

Maximum Sublayer Thickness

The screenshot shows the 'Special Features' tab in a software application. The interface is divided into two sub-tabs: 'Maximum Sublayer Thickness' and 'Radioactive/Biological Decay'.
 In the 'Maximum Sublayer Thickness' sub-tab, there is a warning message: 'Warning: When overriding the default maximum layer thickness the program may crash or give false results.' Below the warning, there is a text input field labeled 'Maximum Layer Thickness:' with the value '10.01'.
 In the 'Radioactive/Biological Decay' sub-tab, there is a list of checkboxes. The 'Radioactive/Biological Decay' checkbox is checked, while all other checkboxes ('Initial Concentration Profile', 'Non-linear Sorption', 'Passive Sink', 'Print Mass in Base', 'Time Varying Properties', 'Monte Carlo Simulation', and 'Sensitivity Analysis') are unchecked.

The Maximum Sublayer Thickness special feature allows the user to override the default maximum sublayer thickness of 5 units. This maximum is set to avoid problems with exponential overflow which can sometimes occur if the sublayers are too large. When overriding the default you take the risk that

the program will crash or give false results - caveat emptor!.

To change the maximum sublayer thickness, check the Maximum Sublayer Thickness box on the tab. On the Maximum Sublayer Thickness sub-tab a value of 10.01 is used, each sublayer may be up to 10.01 m thick in this example. The reason for changing this parameter is to allow the calculation of depth at 10 m intervals in the 50 m layer.

Radioactive/Biological Decay

Maximum Sublayer Thickness Radioactive/Biological Decay

Source Decay: Yes No

Base Decay: Yes No

Source Half-Life: 100 yr Base Half-Life: 100 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	50	m	100	yr

To specify the radioactive decay, check the Radioactive/Biological Decay box on the tab. On the Radioactive/Biological Decay sub-tab the source and base decay can be specified. The data for the depth ranges can also be entered. In this example there is one depth range, corresponding to the entire thickness of the layer, with a half-life of 100 years.

Model Execution



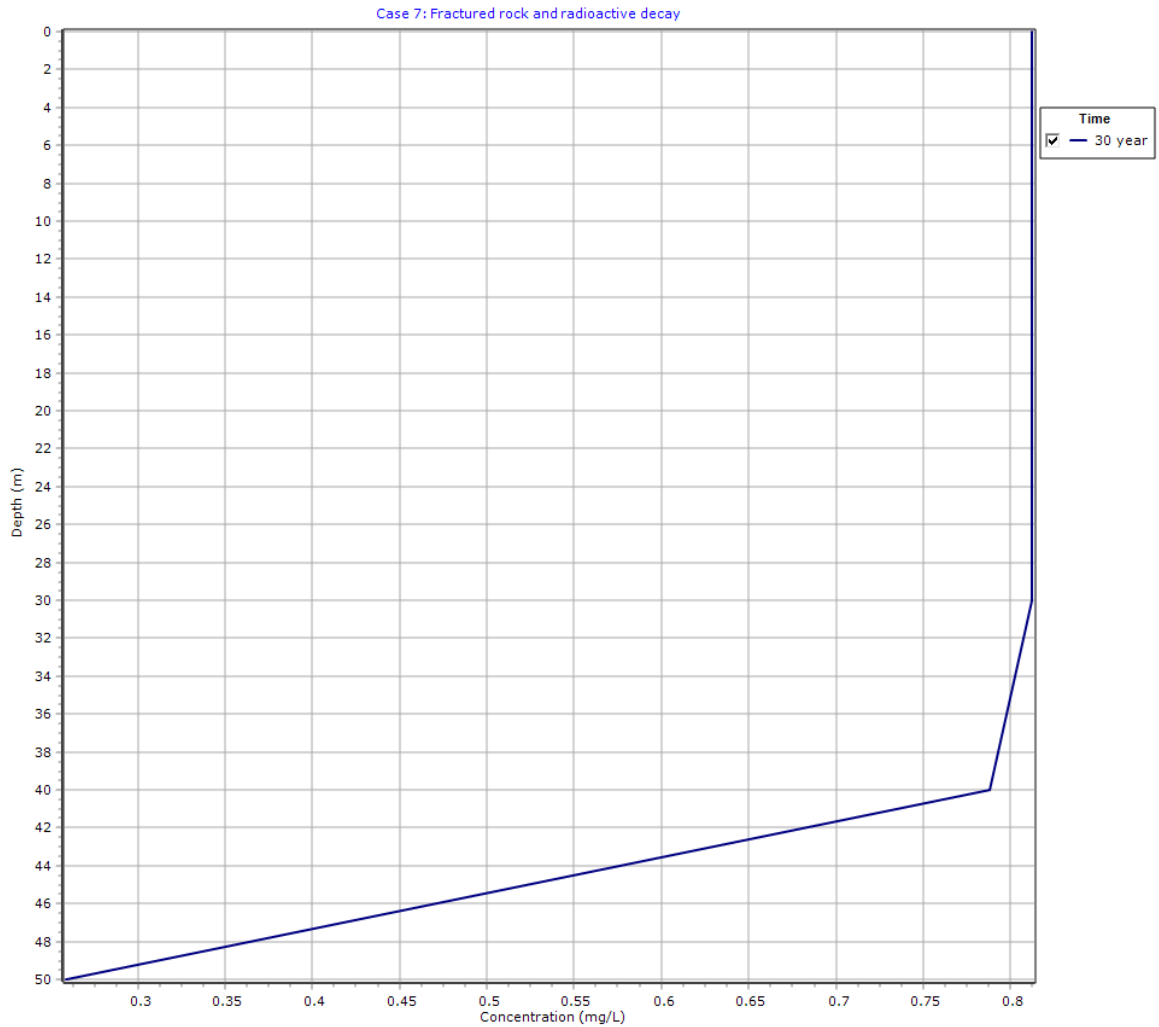
To run the model and calculate the concentrations press the Run button on the toolbar.

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 7: Fractured rock and radioactive decay

THE DARCY VELOCITY (Flux) THROUGH THE LAYERS $V_a = 0.08$ m/year

Layer Properties

Layer	Fracture Spacing 1	Opening Size 1	Number 1	Fracture Spacing 2	Opening Size 2	Number 2	Fracture Spacing 3	Opening Size 3	Number 3
Fractured Rock	0.05 m	1E-5 m	10						

Layer	Dispersion Coefficient in Fractures	Distribution Coefficient in Fractures	Fracture Porosity	Retardation Coefficient in Matrix
Fractured Rock	6 m ² /a	0 m ³ /kg	2.0000E-04	1.0000E+00

Layer	Thickness	Number of Sublayers	Coefficient of Hydrodynamic Dispersion	Matrix Porosity	Distributon Coefficient	Dry Density
Fractured Rock	50 m	5	0.0018 m ² /a	0.05	0 m ³ /kg	2 g/cm ³

Boundary Conditions**Constant Concentration**

Source Concentration = 1 mg/L

Infinite Thickness Bottom Boundary**Radioactive or Biological Decay**

Radioactive or Biological Decay Source Half Life = 100 yr

Radioactive or Biological Decay Base Half Life = 100 yr

First Order Radioactive or Biological Decay Depth Ranges

Minimum Depth	Maximum Depth	Half Life
0 m	50 m	100 yr

Laplace Transform Parameters

TAU = 7 N = 40 SIG = 0 RNU = 4

Calculated Concentrations at Selected Times and Depths

Time year	Depth m	Concentration mg/L
30	0.000E+00	8.123E-01
	1.000E+01	8.123E-01
	3.000E+01	8.123E-01
	4.000E+01	7.881E-01
	5.000E+01	2.588E-01

NOTICE

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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.

Below is the results using the default Laplace Transform parameters. These results are clearly wrong! The other values are correct. We can get the correct value at 50 m by increasing the amount of integration as indicated in the previous output listing.

Calculated Concentrations at Selected Times and Depths

Time year	Depth m	Concentration mg/L
30	0.000E+00	8.123E-01
	1.000E+01	8.123E-01
	3.000E+01	8.123E-01
	4.000E+01	7.883E-01
	5.000E+01	-1.384E+02