POLLUTE

Version 8

Example 12: POLLUTE vs. Analytical Solution

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Description

The results obtained from POLLUTE are compared to those obtained by an analytical solution developed by Tang et al. (1981) for a single fracture system. A conservative contaminant is considered with a constant source concentration of 1. The fractures are 10 µm wide, have a groundwater (seepage) velocity along the fracture of 730 m/a, a dispersivity of zero, and a diffusion coefficient along the fractures of 0.077 m^2/a. In this comparison the fracture spacing is 1 m. Because of the very low matrix diffusion coefficient there is no interaction between fractures over the time frame considered, thus the same result would be obtained if the fracture spacing were increased to 10 m. The Darcy velocity, which occurs along the fractures, can be calculated by multiplying the fractures per m times the fracture width times the seepage velocity:

$$v_a = 10x10^{-6} * 1 * 730 = 0.73x10^{-2}$$

A porosity of 0.05 and tortuosity (the ratio of effective diffusion coefficient to the molecular diffusion coefficient in water) of 0.0000983 were assumed for the matrix material. The matrix diffusion coefficient is then given by multiplying the fracture diffusion coefficient and the tortuosity:

$D_m = 0.077 * 0.0000983 = 7.5691x10^{-6}$

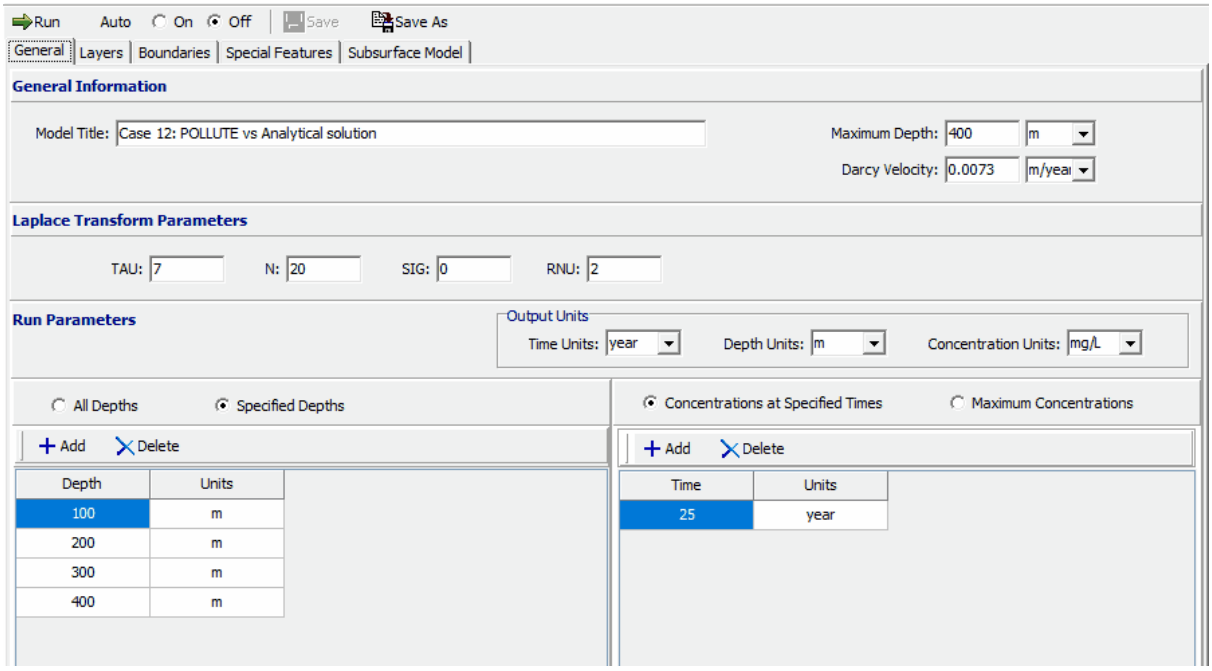
The following parameters are defined for this example:

Property	Symbol	Value	Units
Darcy Velocity	v_a	7.30E-03	m/a
Soil Thickness	H	400	m
Number of Sub-layers		4	-
Fracture spacing	$2H_1$	1	m
Fracture opening	$2h_1$	10E-6	m
Dispersion along fractures	D_f	0.077	m^2/a
Fracture Distribution Coef.	K^f	0	cm^3/g
Matrix Diffusion Coefficient	D_m	7.57E-6	m^2/a
Matrix Distribution Coef.	K_m	1	cm^3/g
Matrix Porosity	n_m	0.05	-
Dry Density of Matrix		0	g/cm^3
Source Concentration	c_0	1	mg/L

Data Entry

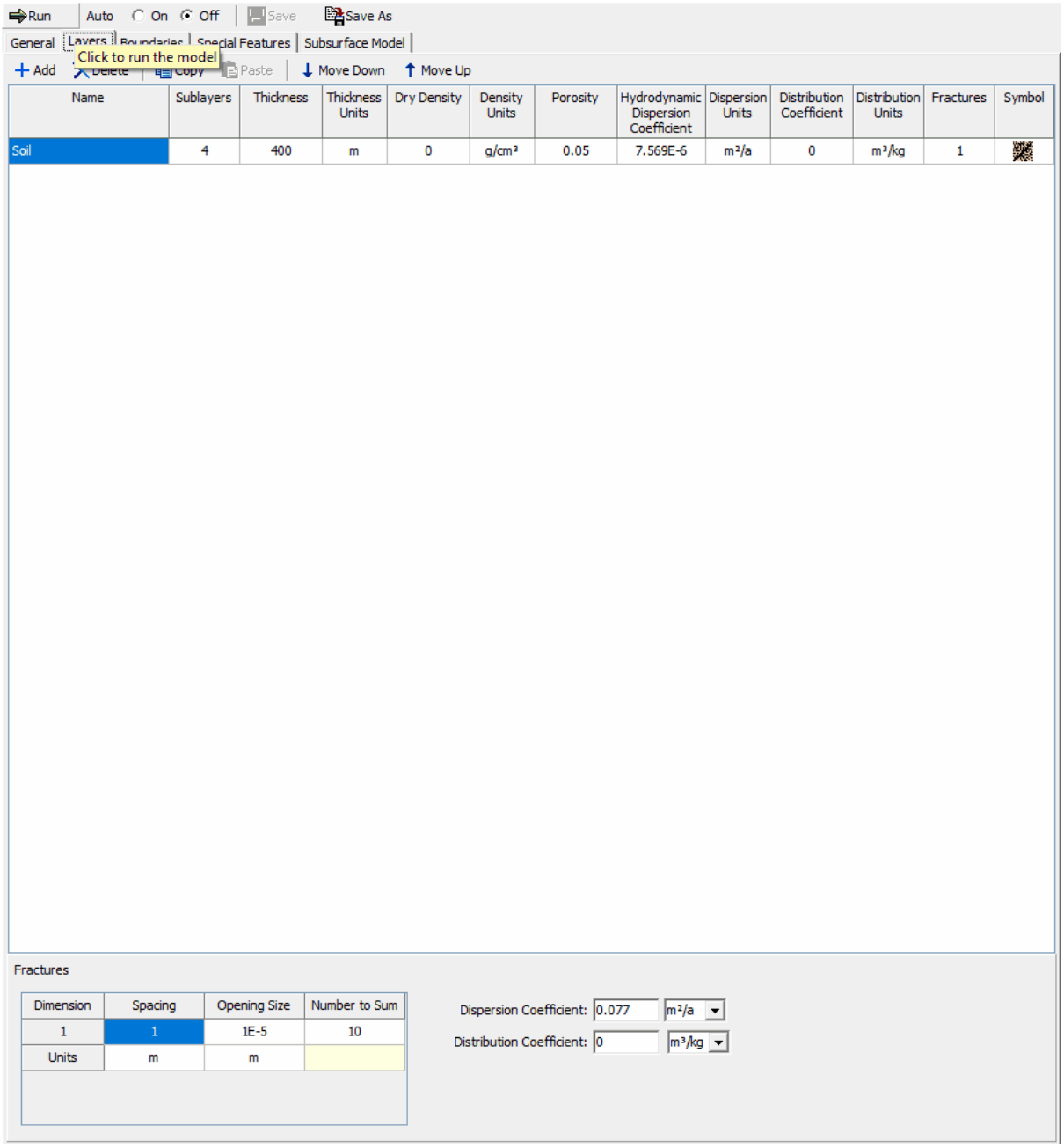
Open the Examples project and open Case 12.

General Tab



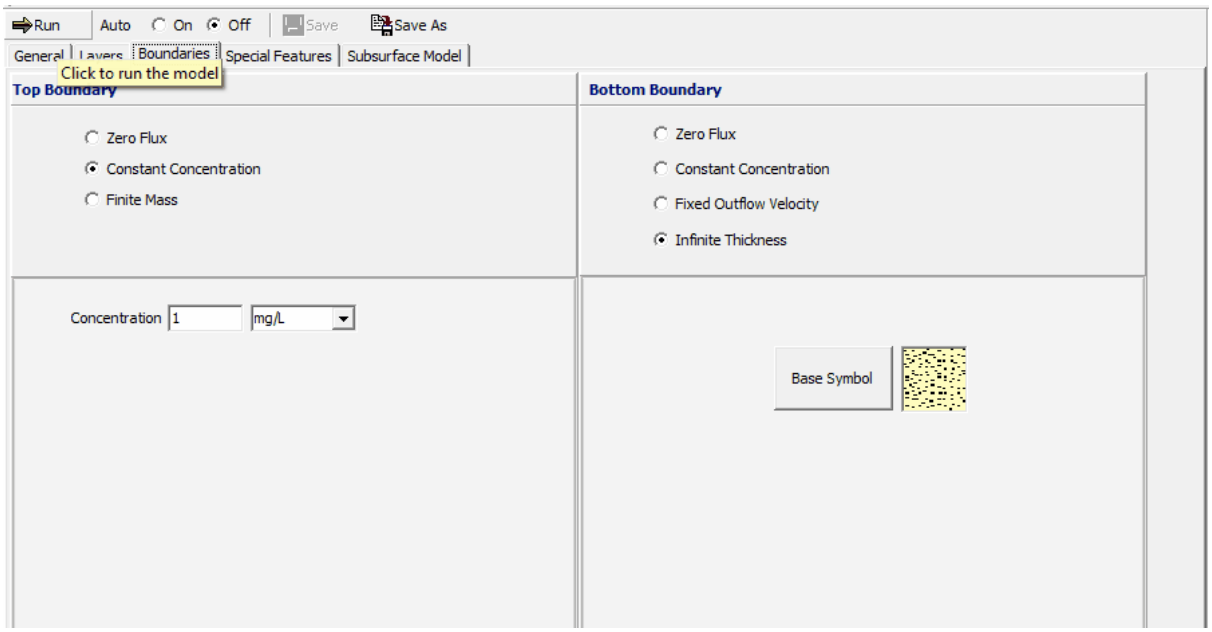
The general data for this example can be specified on the General tab. The Darcy velocity can be specified as 0.73×10^{-2}. The Run Parameters can be specified at the bottom of the tab. In this example the concentrations will be calculated at 25 years and at 4 depths: 100, 200, 300, and 400 m.

Layers Tab



The layer data for the layer can be specified on the Layers tab. The data for the one dimensional fractures can be specified when the layer is selected. The fracture opening size is the gap between the walls of the fracture.

Boundaries Tab



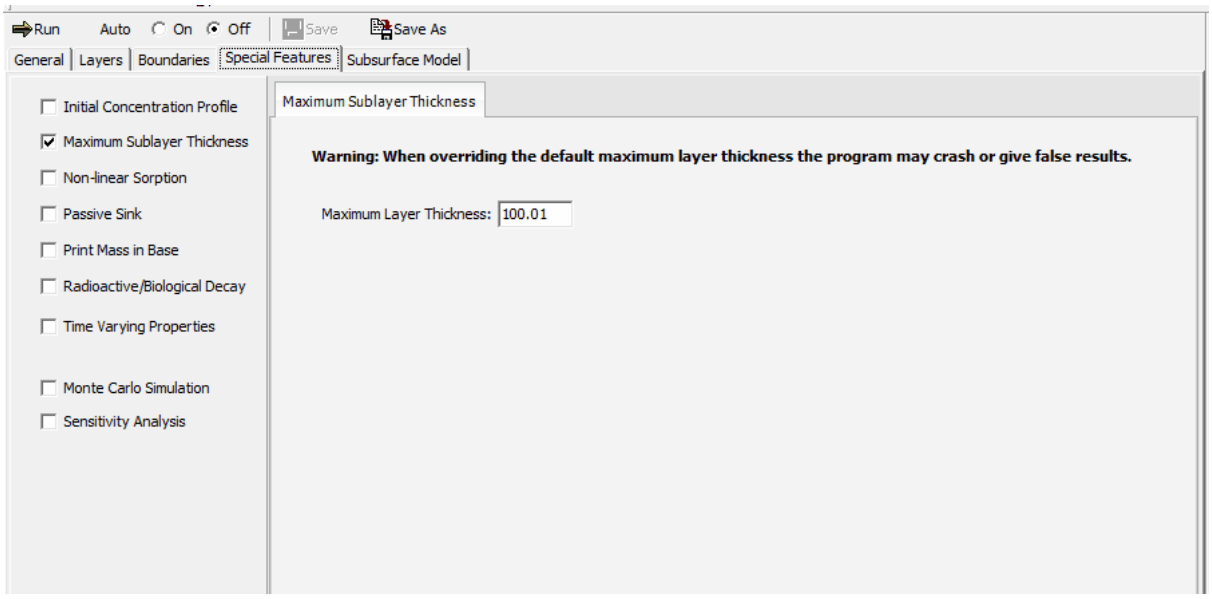
The boundary conditions for the model can be specified on the Boundaries tab. In this example, the top boundary has a constant concentration and the bottom boundary is represented by a layer of infinite thickness.

Special Features

The maximum sublayer thickness for this example can be specified using the Special Features tab.

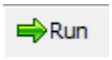
Maximum Sublayer Thickness

The default maximum sublayer thickness is 5 depth units. This maximum is set to avoid problems with exponential overflow, which can sometimes occur if the sublayers are too thick. To override the default maximum sublayer thickness the Maximum Sublayer Thickness feature is used, when over riding this default the user takes the chance that the program will “crash” or give false results - caveat emptor.



To specify the maximum sublayer thickness check the Maximum Sublayer Thickness box item from the Special Features tab, By specifying the maximum sublayer thickness as 100.01 the sublayers can be up to 100.01 units thick. In this example the sublayers are 100 units thick.

Model Execution



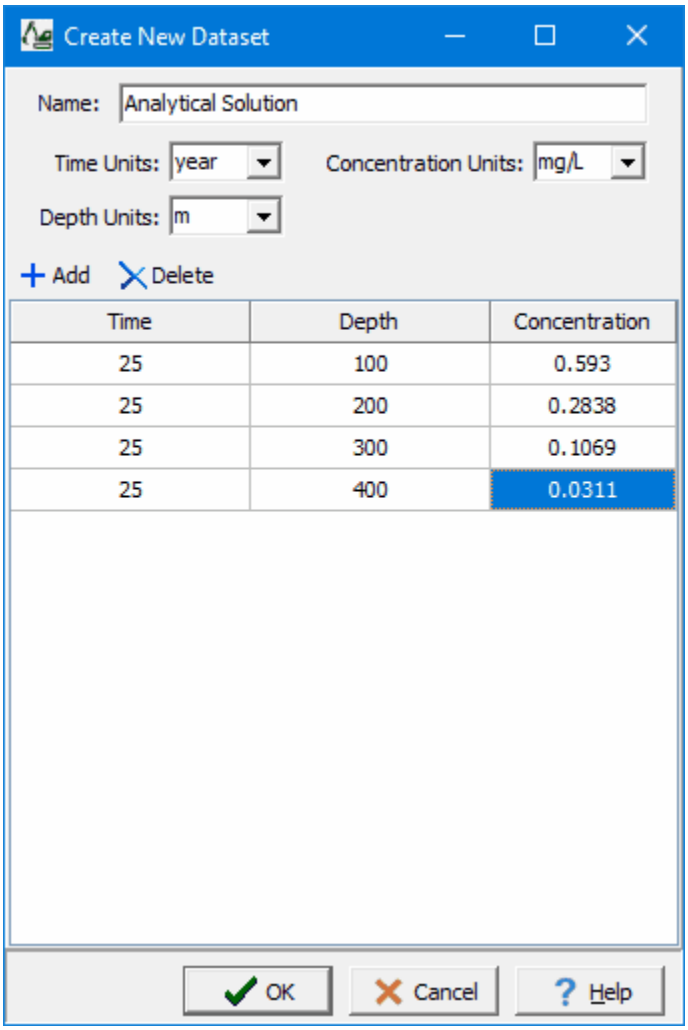
To run the model and calculate the concentrations press the Run button on the toolbar.

Model Output

After the model has been executed, the output for the model will be displayed.

Output Comparison

The results given by analytical solution can be compared to the output by creating a new imported dataset using *File > New > Imported Dataset*.

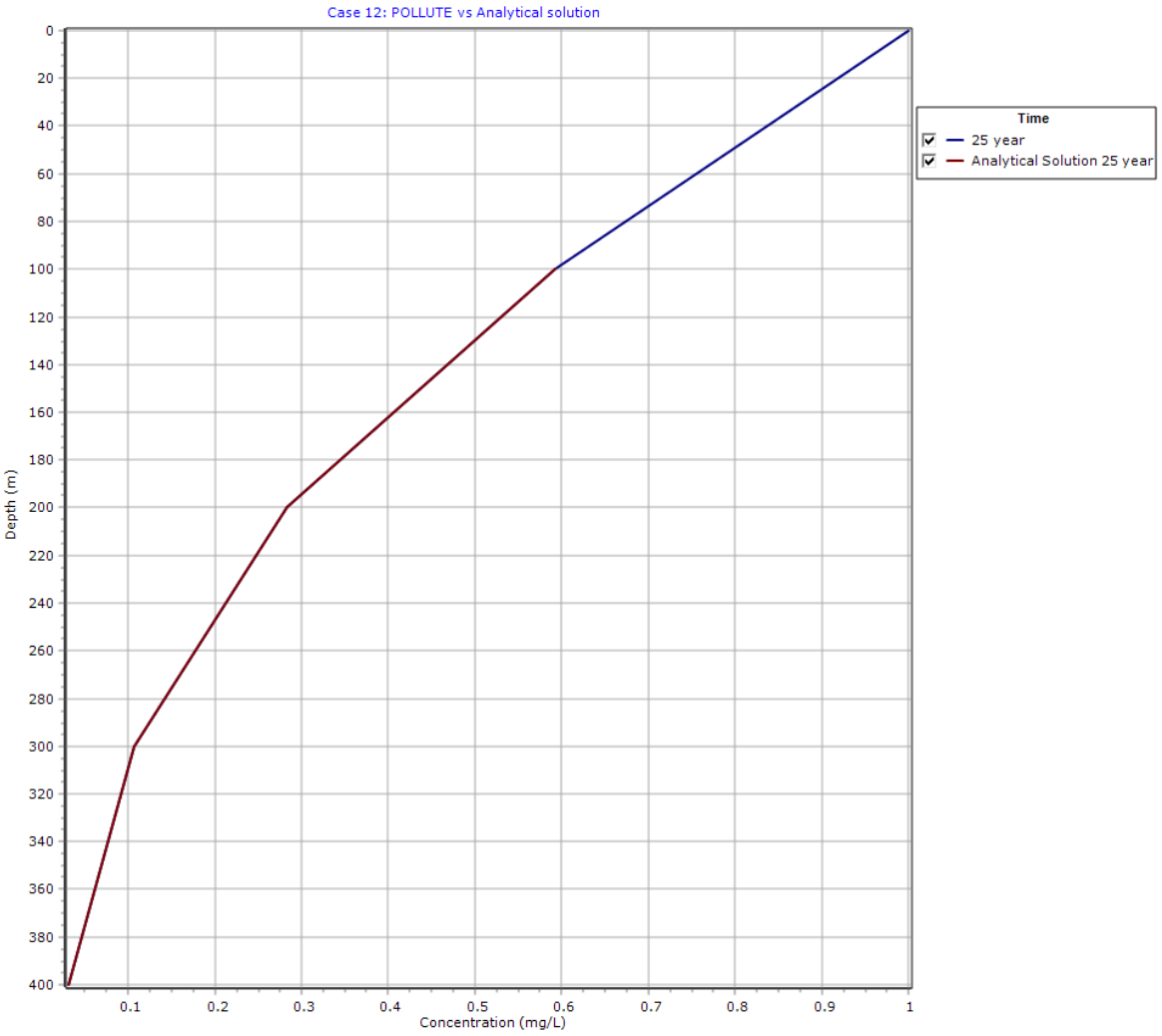


The calculated concentrations from the POLLUTE program and the analytical solution by Tang et al. (1981) are listed below. Both solutions give identical results.

Depth	**POLLUTE**	**Analytical Solution**
(m)	(mg/L)	(mg/L)
100	0.593	0.593
200	0.2838	0.2838
300	0.1069	0.1069
400	0.0311	0.0311

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.

POLLUTEv8

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Case 12: POLLUTE vs Analytical solution

THE DARCY VELOCITY (Flux) THROUGH THE LAYERS Va = 0.0073 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
Soil	1 m	1E-5 m	10						

Layer	Dispersion Coefficient in Fractures	Distribution Coefficient in Fractures	Fracture Porosity	Retardation Coefficient in Matrix
Soil	0.077 m²/a	0 m³/kg	1.0000E-05	1.0000E+00

Layer	Thickness	Number of Sublayers	Coefficient of Hydrodynamic Dispersion	Matrix Porosity	Distributon Coefficient	Dry Density
Soil	400 m	4	7.569E-6 m²/a	0.05	0 m³/kg	0 g/cm³

Boundary Conditions

Constant Concentration

Source Concentration = 1 mg/L

Infinite Thickness Bottom Boundary

Laplace Transform Parameters

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

Calculated Concentrations at Selected Times and Depths

Time year	Depth m	Concentration mg/L
25	0.000E+00	1.000E+00
	1.000E+02	5.930E-01
	2.000E+02	2.838E-01
	3.000E+02	1.069E-01
	4.000E+02	3.111E-02