Created in COMSOL Multiphysics 6.0

Solute Transport in Prescribed Groundwater Flow

Introduction

This model tracks a solute in a prescribed groundwater flow over 1000 days accounting for longitudinal and transversal dispersivity.

This set up is often used as a benchmark case to verify different implementations for modeling species transport. It compares the results with an analytical solution (Ref. 1).

Model Definition

The model geometry is a square with a side length of 4 km. Because the groundwater flow is prescribed, the model solves for species transport only with a predefined flow field of magnitude $0.5\sqrt{2}\ \mathrm{m/d}$.

An initial concentration following a Gaussian distribution is applied. The analytical solution can be defined as a function in COMSOL. See Ref. 1 for the analytical expression. Because this expression is quite long and just used to compare the simulation results against it, a preset file is loaded that contains the analytical solution already (Figure 1).

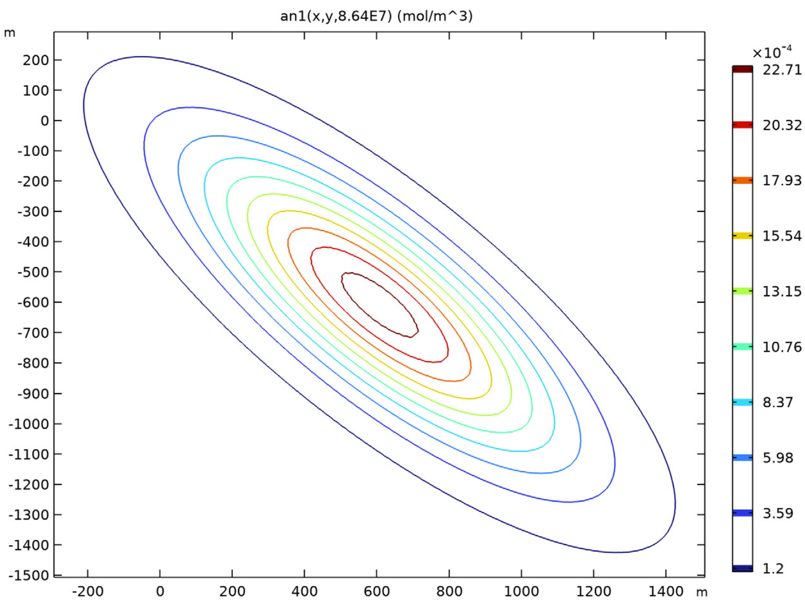


Figure 1: Analytical solution for the concentration after 1000 days.

Results and Discussion

Figure 2 shows the result after 1000 days. The predefined flow field is visualized by an arrow streamline plot. The analytical solution is also plotted (white contour lines) and it can be seen that the simulation results (filled contours) matche the analytical solution.

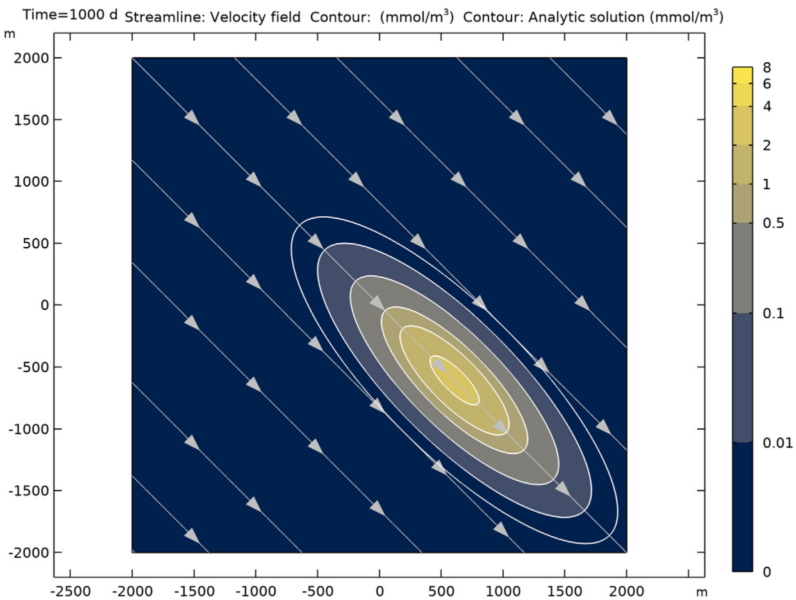


Figure 2: Resulting concentration distribution after 1000 days (filled contours) compared with the analytical solution (white contours). Arrow streamlines visualize the prescribed flow direction.

Reference

1. J.L. Wilson and P.J. Miller, "Two-dimensional plume in uniform ground-water flow," *Journal of the Hydraulics Division*, ASCE, 1978.

Application Library path: `Subsurface_Flow_Module/Solute_Transport/solute_transport`

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

2 In the **Application Libraries** window, select **Subsurface Flow Module>Solute Transport>solute_transport_preset** in the tree.

3 Click **Open**.

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **2D**.

GEOMETRY 1

Square 1 (sq1)

1 In the **Geometry** toolbar, click **Square**.

2 In the **Settings** window for **Square**, locate the **Size** section.

3 In the **Side length** text field, type `L`.

4 Locate the **Position** section. From the **Base** list, choose **Center**.

5 Click **Build All Objects**.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Chemical Species Transport>Transport of Diluted Species in Porous Media (tds)**.

4 Click **Add to Component 1** in the window toolbar.

5 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Transport of Diluted Species in Porous Media (tds)>Porous Medium 1** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Convection** section.

3 Specify the **u** vector as

u	x
v	y

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.

3 From the ε_p list, choose **User defined**. In the associated text field, type `ne`.

Porous Medium 1

In the **Model Builder** window, click **Porous Medium 1**.

Dispersion 1

1 In the **Physics** toolbar, click **Attributes** and choose **Dispersion**.

2 In the **Settings** window for **Dispersion**, locate the **Dispersion** section.

3 From the **Dispersion tensor** list, choose **Dispersivity**.

4 In the α_L text field, type `aL`.

5 In the α_T text field, type `aT`.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundaries 1 and 3 only.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundaries 2 and 4 only.

The source term is defined as initial value. First, define the 2D Gauss distribution as a function.

DEFINITIONS

Analytic 2 (an2)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, type `gaussian` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `1/(2*pi*esrc^2)*exp(-(x^2+y^2)/(2*esrc^2))`.

4 In the **Arguments** text field, type `x, y`.

5 Locate the **Units** section. In the table, enter the following settings:

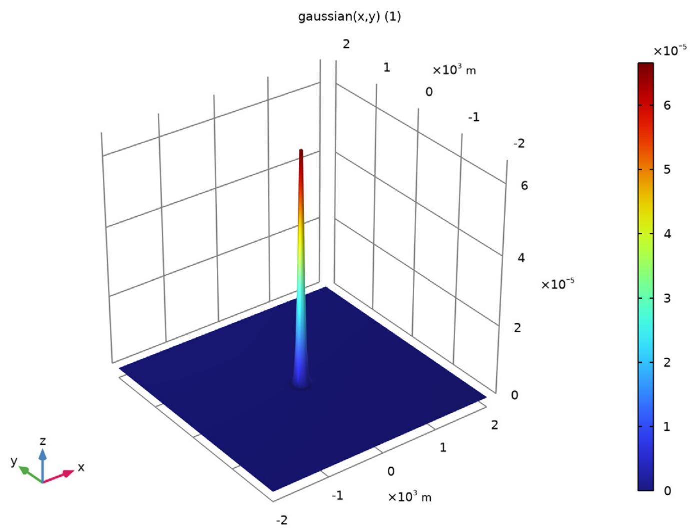
Argument	**Unit**
x	m

6 In the **Function** text field, type `1`.

7 Locate the **Plot Parameters** section. In the table, enter the following settings:

Argument	**Lower limit**	**Upper limit**	**Unit**
x	-2000	2000	m
y	-2000	2000	

8 Click **Plot**.



TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species in Porous Media (tds)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *c* text field, type `M*gaussian(x-x0,y-y0)`.

Define a variable for the analytical solution which makes it easier to compare the results in postprocessing.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
c_analytic	an1(x,y,t)	mol/m³	Analytic solution

To resolve the spatial distribution, a fine mesh is required. Use a mapped mesh.

MESH 1

Mapped 1

In the **Mesh** toolbar, click **Mapped**.

Size

1 In the **Model Builder** window, click **Size**.

2 In the **Settings** window for **Size**, click to expand the **Element Size Parameters** section.

3 In the **Maximum element size** text field, type 20.

4 Click **Build All**.

Add a time-dependent study to run the simulation over 1000 days. Restrict the maximum time step, for an accurate solution.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 1

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 From the **Time unit** list, choose **d**.

3 In the **Output times** text field, type `range(0,100,1000)`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

4 From the **Maximum step constraint** list, choose **Constant**.

5 In the **Maximum step** text field, type `20`.

6 Click **Compute**.

RESULTS

Concentration (tds)

To create Figure 2 proceed as follows.

Concentration compared

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Concentration compared` in the **Label** text field.

Streamline 1

1 Right-click **Concentration compared** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Transport of Diluted Species in Porous Media>tds.u,tds.v - Velocity field**.

3 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Uniform density**.

4 In the **Separating distance** text field, type `0.1`.

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **Gray**.

6 From the **Type** list, choose **Arrow**.

Contour 1

1 In the **Model Builder** window, right-click **Concentration compared** and choose **Contour**.

2 In the **Settings** window for **Contour**, locate the **Expression** section.

3 In the **Unit** field, type `mmol/m^3`.

4 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.

5 In the **Levels** text field, type `0.001 0.01 0.1 0.5 1 2 4 6 8`.

6 Locate the **Coloring and Style** section. From the **Contour type** list, choose **Filled**.

7 From the **Color table** list, choose **Cividis**.

8 From the **Scale** list, choose **Logarithmic**.

Contour 2

1 Right-click **Concentration compared** and choose **Contour**.

2 In the **Settings** window for **Contour**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>c_analytic - Analytic solution - mol/m³**.

3 Locate the **Expression** section. In the **Unit** field, type `mmol/m^3`.

4 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.

5 In the **Levels** text field, type `0.001 0.01 0.1 0.5 1 2 4 6 8`.

6 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

7 From the **Color** list, choose **White**.

8 Clear the **Color legend** check box.

9 In the **Concentration compared** toolbar, click **Plot**. Compare with Figure 2.