Created in COMSOL Multiphysics 5.3a

# 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)

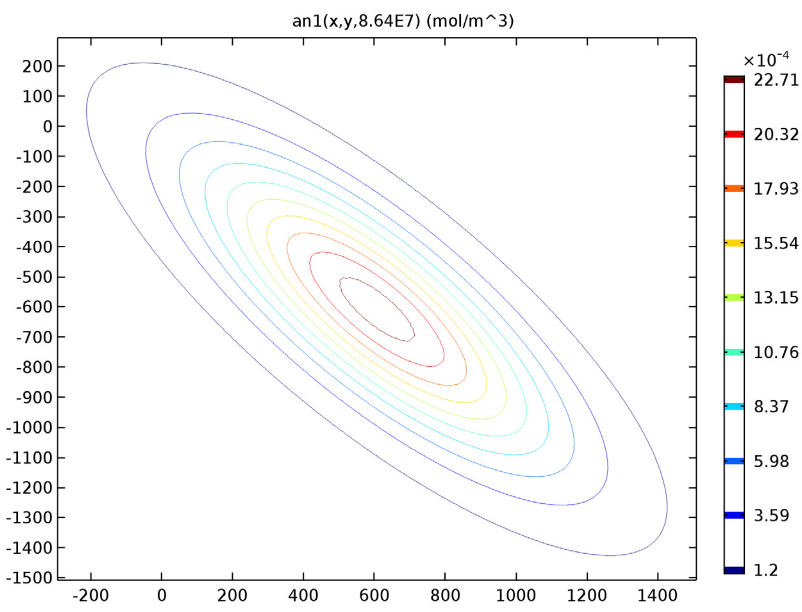



*Figure 1: Analytical solution for the concentration after 1000 days.*

## Results and Discussion

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

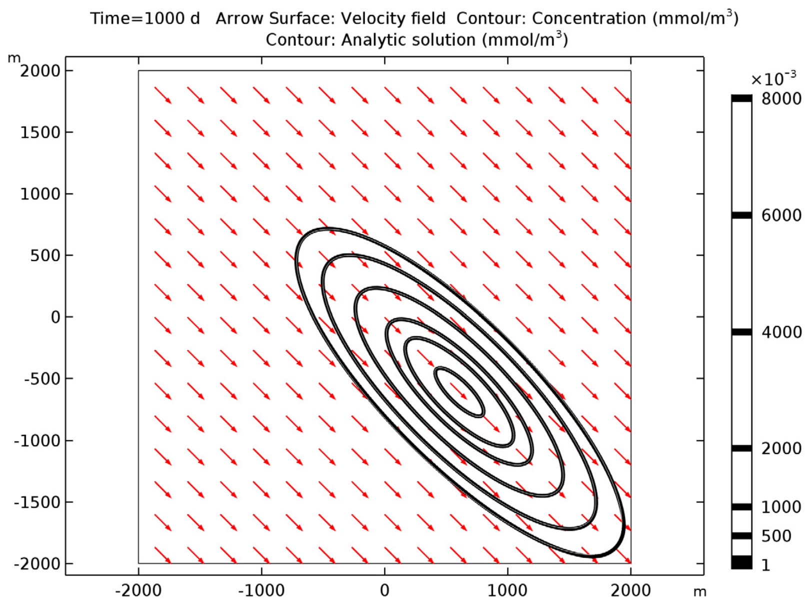



*Figure 2: Resulting concentration distribution after 1000 days (black contours) compared with the analytical solution (white contours). Red arrows visualize the prescribed flow direction.*

## 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`

### ROOT

1 From the **File** menu, choose **Open**.

2 Browse to the model's Application Libraries folder and double-click the file `solute_transport_preset.mph`.

### RESULTS

*Surface 1*

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

### GEOMETRY 1

*Square 1 (sq1)*

1 On the **Geometry** toolbar, click **Primitives** and choose **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**.

### COMPONENT 1 (COMP1)

On the **Home** toolbar, click **Windows** and choose **Add Physics**.

### ADD PHYSICS

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

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

3 Click **Add to Component** in the window toolbar.

### TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

1 In the **Settings** window for **Transport of Diluted Species in Porous Media**, locate the **Transport Mechanisms** section.

2 Find the **Porous media transport** subsection. Select the **Dispersion** check box.

*Porous Media Transport Properties 1*

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

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

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

4 Locate the **Convection** section. Specify the **u** vector as

| | |
|---|---|
| u | x |
| v | y |

5 Locate the **Dispersion** section. From the **Dispersion tensor** list, choose **Dispersivity**.

6 In the $\alpha_L$ text field, type `aL`.

7 In the $\alpha_T$ text field, type `aT`.

*Inflow 1*

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

2 Select Boundaries 1 and 3 only.

*Outflow 1*

1 On 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 On the **Home** toolbar, click **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`.

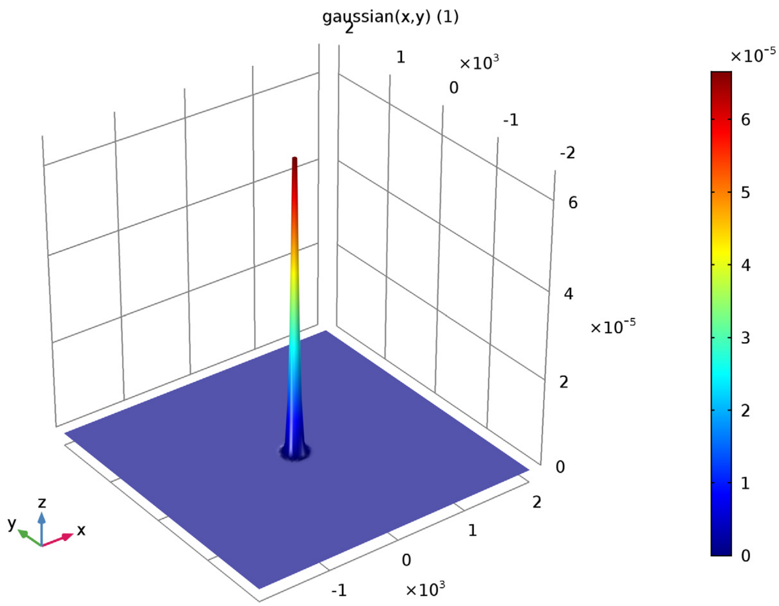
5 Locate the **Units** section. In the **Arguments** text field, type `m`.

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 |
|---|---|---|
| x | -2000 | 2000 |
| 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

*Size*

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

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

3 Locate the **Element Size Parameters** section. 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 On 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 **Preset Studies>Time Dependent**.

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

### 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 **Times** text field, type `range(0,100,1000)`.

### *Solution 1 (sol1)*

1. On 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. Locate the **Time Stepping** section. Select the **Maximum step** check box.
5. In the associated text field, type `20`.
6. Click **Compute**.

## RESULTS

### *Concentration (tds)*

To create Figure 2 proceed as follows.

### *2D Plot Group 3*

1. On 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.

### *Arrow Surface 1*

1. Right-click **Concentration compared** and choose **Arrow Surface**.
2. In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Transport of Diluted Species in Porous Media>tds.u,tds.v - Velocity field**.

### *Contour 1*

1. In the **Model Builder** window, under **Results** 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 **Tube**.
7. From the **Coloring** list, choose **Uniform**.
8. From the **Color** list, choose **Black**.

*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>Definitions>Variables>c_analytic - Analytic solution**.
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 On the **Concentration compared** toolbar, click **Plot**.