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 $0.5\sqrt{2}$ 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.](image-url)
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


Application Library path: Subsurface_Flow_Module/Solute_Transport/solute_transport
Modeling Instructions

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 \( \mathbf{u} \) vector as

\[
\begin{align*}
\mathbf{u} & \quad x \\
\mathbf{v} & \quad y
\end{align*}
\]

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>A nalytic.

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

<table>
<thead>
<tr>
<th>Argument</th>
<th>Lower limit</th>
<th>Upper limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>-2000</td>
<td>2000</td>
</tr>
<tr>
<td>y</td>
<td>-2000</td>
<td>2000</td>
</tr>
</tbody>
</table>

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 * text field, type $M*\text{gaussian}(x-x0, y-y0)$.

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

Variables

1 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:

<table>
<thead>
<tr>
<th>Name</th>
<th>Expression</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>c_analytic</td>
<td>an1(x,y,t)</td>
<td>mol/m³</td>
<td>Analytic solution</td>
</tr>
</tbody>
</table>

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**.

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.