Solute Injection

Introduction

This is a benchmark case for modeling transport of contaminants through an aquifer. First a stationary Darcy flow field is computed and followed up by a transient species transport simulation. The results are compared to the benchmark situation (Ref. 1).

In addition, this model shows how to use the adaptive mesh refinement algorithm to obtain a proper mesh which resolves the given problem accurately.

Model Definition

The model geometry is depicted below.

Figure 1: Geometry for the benchmark case.

The contaminant source is located at $x = y = 150\ \mathrm{m}$. The benchmark assumes an aquifer thickness of $b = 10$ m. To take this thickness in to account and compare the solutions all source terms will be scaled by this value.

FLUID FLOW

Darcy's Law is used to compute the flow field. Constant heads on the left and right hand side are applied. At the top and bottom boundary no flow condition is used. Water with density ρ_f is pumped at a rate $W = 1$ m³/d into the aquifer. A mass flux of $N_0 = \rho_f W/b$ is applied as point source.

CONTAMINANT TRANSPORT

The contaminant is transported by convection, diffusion, and dispersion. The relation of longitudinal to transverse dispersivity is 10 to 3.

On the left boundary a fixed concentration $c = 0$ is applied to reproduce the benchmark case. All other boundaries are defined as outflow boundaries. The species concentration c_0 at the source is 1 kg/m^3. A molar mass of M = 1 g/mol is assumed to obtain a molar concentration of 1000 mol/m^3. Hence, the mass source at the point is defined according to $q = c_0 W/(\mathrm{Mb})$.

Results and Discussion

The stationary flow field is shown in Figure 2. As expected the flow field itself is almost unaffected by the point source.

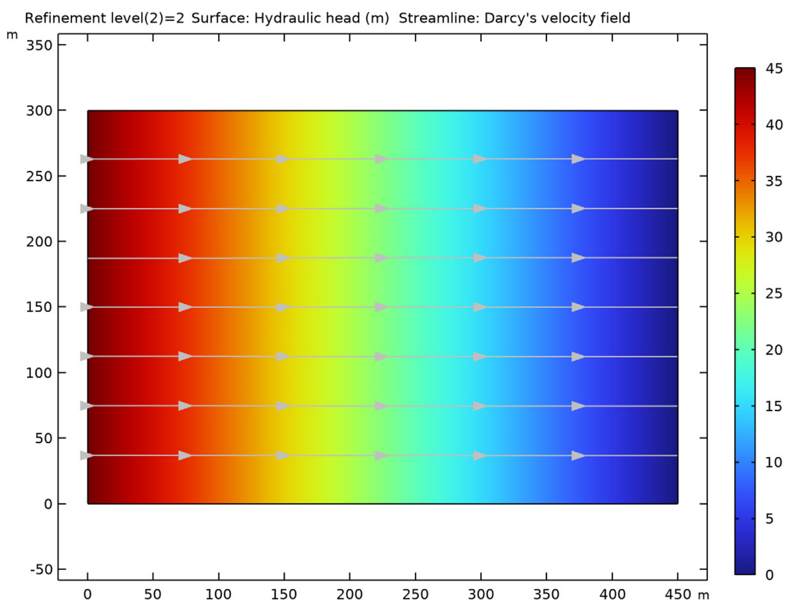


Figure 2: Stationary Darcy velocity field and hydraulic head.

Figure 3 and Figure 4 show different plots for the concentration distribution after 360 days.

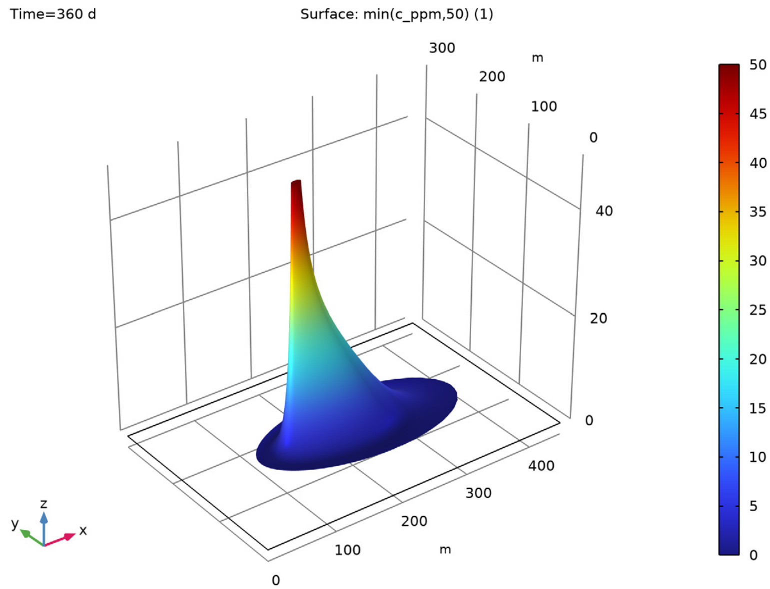


Figure 3: Concentration distribution after 360 days.

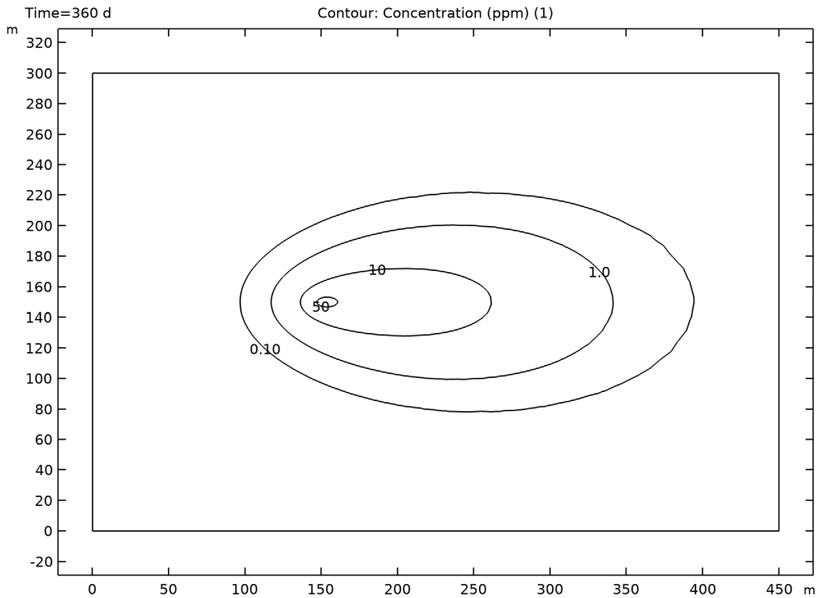


Figure 4: Concentration contours after 360 days.

Notes About the COMSOL Implementation

This model makes use of the adaptive mesh refinement algorithm to get a proper mesh resolution. It is based on an error estimation such that regions with strong gradients, like the point source will be resolved with finer mesh elements than regions with small gradients.

Reference

1. C. Zheng and P. Wang, *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems*, University of Alabama, 1998.

Application Library path: `Subsurface_Flow_Module/Verification_Examples/solute_injection`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow>Darcy's Law (dl)**.

3 Click **Add**.

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

5 Click **Add**.

6 Click **Study**.

7 In the **Select Study** tree, select **General Studies>Stationary**.

8 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
W	1[m^3/d]	1.1574E-5 m³/s	Pumping rate
b	10[m]	10 m	Aquifer thickness
H_in	45[m]	45 m	Inlet head
rho_f	1000[kg/m^3]	1000 kg/m³	Fluid density
c0	1[kg/m^3]	1 kg/m³	Concentration at source
M	1[g/mol]	0.001 kg/mol	Molar mass
c_in	c0/M	1000 mol/m³	Concentration at source

GEOMETRY 1

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.
2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3 In the **Width** text field, type `450`.
4 In the **Height** text field, type `300`.

Point 1 (pt1)

1 In the **Geometry** toolbar, click **Point**.
2 In the **Settings** window for **Point**, locate the **Point** section.
3 In the **x** text field, type `150`.
4 In the **y** text field, type `150`.
5 Click **Build All Objects**.

DARCY'S LAW (DL)

Porous Matrix 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law (dl)> Porous Medium 1** click **Porous Matrix 1**.
2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.
3 From the **Permeability model** list, choose **Hydraulic conductivity**.
4 In the K text field, type `1[m/d]`.

Hydraulic Head 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Hydraulic Head**.
2 Select Boundary 1 only.
3 In the **Settings** window for **Hydraulic Head**, locate the **Hydraulic Head** section.
4 In the H_0 text field, type `H_in`.

Hydraulic Head 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Hydraulic Head**.
2 Select Boundary 4 only.

Line Mass Source 1

1 In the **Physics** toolbar, click **Points** and choose **Mass Source**.
2 Select Point 3 only.

3 In the **Settings** window for **Line Mass Source**, locate the **Line Mass Source** section.

4 In the N_0 text field, type `W/b*rho_f`.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Use quadratic shape functions. This results in a smoother solution.

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

2 In the **Settings** window for **Transport of Diluted Species in Porous Media**, click to expand the **Discretization** section.

3 From the **Concentration** list, choose **Quadratic**.

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 From the $\mathbf{u}$ list, choose **Darcy's velocity field (dl/porous1)**.

4 Locate the **Diffusion** section. From the **Effective diffusivity model** list, choose **No correction**.

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 Select the **Specify dispersion for each species individually** check box.

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

5 In the $\alpha_{L,c}$ text field, type `10`.

6 In the $\alpha_{T,c}$ text field, type `3`.

Concentration 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species c** check box.

Outflow 1

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

2 Select Boundaries 2–4 only.

Line Mass Source 1

1 In the **Physics** toolbar, click **Points** and choose **Line Mass Source**.

2 Select Point 3 only.

3 Type `c_in*W/b`.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	rho_f	kg/m³	Basic
Porosity	epsilon	0.3	1	Basic

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_ppm	c*M*1e6/rho_f		Concentration (ppm)

MESH 1

To build a proper mesh that resolves the strong gradients at the point use an adaptive mesh refinement algorithm. First, change the mesh resolution to finer. This is the initial mesh.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Finer**.

STUDY 1

Step 1: Stationary

Calculate the stationary Darcy flow field with adaptive mesh refinement.

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Transport of Diluted Species in Porous Media (tds)**.

4 Click to expand the **Adaptation and Error Estimates** section. From the **Adaptation and error estimates** list, choose **Adaptation and error estimates**.

5 Clear the **Save solution on every adapted mesh** check box.

This saves the solution on the final mesh only.

6 Find the **Mesh adaptation** subsection. From the **Adaptation method** list, choose **Rebuild mesh**.

This means that a completely new mesh is built.

7 In the **Home** toolbar, click **Compute**.

RESULTS

Hydraulic Head

A pressure plot and a concentration plot are created by default. Modify the pressure plot to display the hydraulic head and velocity field as in Figure 2.

1 In the **Model Builder** window, under **Results** click **Pressure (dl)**.

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

Surface

1 In the **Model Builder** window, expand the **Hydraulic Head** node, then click **Surface**.

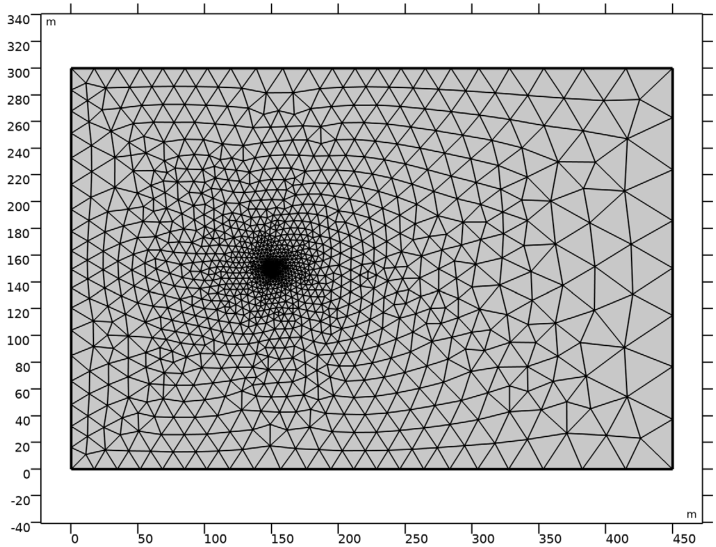
2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Darcy's Law>Velocity and pressure>dl.H - Hydraulic head - m**.

The velocity field is almost homogeneous. This means that the point source term does not disturb the flow field much (see Figure 2).

COMPONENT 1 (COMP1)

Investigate the different mesh levels. You can find them under the **Meshes** node.

LEVEL 2 ADAPTED MESH 2



The **Level 2 Refined Mesh 2** resolves the point source very well.

Now, run the time dependent solute transport on the finest mesh.

1 From the **Home** menu, choose **Add Study**.

ADD STUDY

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

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

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Darcy's Law (dl)**.

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

5 From the **Home** menu, choose **Add Study**.

STUDY 2

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(0,10,365)`.

4 Click to expand the **Mesh Selection** section. The refined mesh is selected automatically.

5 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

6 From the **Method** list, choose **Solution**.

7 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

8 From the **Method** list, choose **Solution**.

9 From the **Study** list, choose **Study 1, Stationary**.

10 In the **Model Builder** window, expand the **Component 1 (comp1)>Meshes** node.

11 Right-click **Study 2** and choose **Compute**.

RESULTS

Modify the concentration plot to reproduce Figure 3.

Streamline 1

1 In the **Model Builder** window, expand the **Concentration (tds)** node.

2 Right-click **Results>Concentration (tds)>Streamline 1** and choose **Delete**.

Surface 1

1 In the **Model Builder** window, under **Results>Concentration (tds)** click **Surface 1**.

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

3 In the **Expression** text field, type `min(c_ppm,50)`.

4 Click to expand the **Range** section. Select the **Manual data range** check box.

5 In the **Minimum** text field, type `0.1`.

6 In the **Maximum** text field, type `50`.

7 In the **Concentration (tds)** toolbar, click **Plot**.

Height Expression 1

Right-click **Surface 1** and choose **Height Expression**.

Create the contour plot as in Figure 4 with the following steps.

Concentration Contours

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 Contours` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 6 (sol6)**.

Contour 1

1 Right-click **Concentration Contours** 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_ppm - Concentration (ppm)**.

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

4 In the **Levels** text field, type `0.1 1 10 50`.

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

6 From the **Color** list, choose **Black**.

7 Select the **Level labels** check box.

8 In the **Precision** text field, type `2`.

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

10 In the **Concentration Contours** toolbar, click **Plot**.