Buoyancy Flow with Darcy's Law—The Elder Problem

Introduction

Density variations can initiate flow even in a still fluid. In earth systems, density variations can arise from naturally occurring salts, subsurface temperature changes, or migrating pollution. This buoyant or density-driven flow factors into fluid movement in salt-lake systems, saline-disposal basins, dense contaminant and leachate plumes, and geothermal reservoirs, to name just a few.

This example duplicates a benchmark problem for time-dependent buoyant flow in a porous medium. Known as the Elder problem (Ref. 1), it follows a laboratory experiment to study thermal convection. When Voss and Souza (Ref. 2) recast the Elder problem for salt concentrations, it became a benchmark that many researchers have used to test a number of variable-density flow codes including SUTRA (Ref. 3) and SEAWAT (Ref. 4).

This application examines the Elder problem for concentrations through a 2-way coupling of two physics interfaces: Darcy's Law and Transport of Diluted Species in Porous Media.

Model Definition

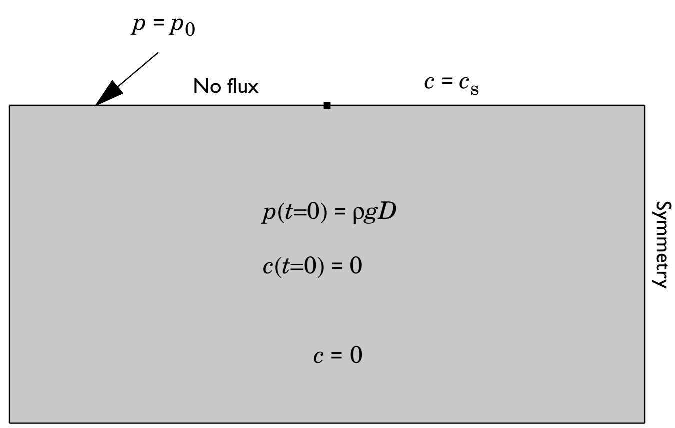

Figure 1: Geometry for modeling the Elder problem with initial conditions and boundary conditions indicated. In this cross section of a water-saturated porous medium, high salt concentrations exist in the top-right region.

In this example (Figure 1) a vertical cross section of a water-saturated porous medium extends 300 m in the x direction and 150 m in the y direction. The material properties are homogeneous and isotropic. A vertical line at $x = 300$ m represents a symmetry boundary with a mirror image of the cross section extending beyond it. There is no flow across the geometry edges. High salt concentrations exist at the upper boundary (along $y = 150$ m) from $x = 150$ m to 300 m. Salt concentration is zero along the lower boundary. The water is initially stationary (with a hydrostatic pressure distribution) and pristine (zero salt concentration). When the density increases near the high-concentration boundary, flow develops. The period of interest is 20 years. According to Ref. 6 and Ref. 7, the length chosen by Elder is close to a critical value that separates downwelling and upwelling plume structures. As a consequence, the problem is particularly sensitive to perturbations.

FLUID FLOW

You can describe the fluid flow in this problem using Darcy's law:

$$\frac{\partial \varepsilon\rho}{\partial t} + \nabla \cdot \rho\mathbf{u} = 0$$

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p + \rho g \nabla D)$$

Here, ρ is the water density (kg/m^3), t is the time (s), ε is the porosity, and $\mathbf{u}$ is the vector of directional seepage rates, also known as the Darcy velocity. The Darcy velocity $\mathbf{u}$ depends on the permeability κ (m^2), the fluid's dynamic viscosity μ (Pa·s), the fluid's pressure p (Pa), and the acceleration of gravity g (m/s^2). The gradient of the elevation D (m) indicates the direction of the vertical coordinate, y.

In Elder's problem, the fluid density depends linearly on the salt concentration, c (mol/m^3) according to

$$\rho = \rho_0 + \beta c = \rho_0 + \frac{\rho_s - \rho_0}{c_s - c_0} c$$

Here, c_0 and c_s are the normalized salt concentrations of pristine and salty water.

The symmetry or zero flow on all boundaries fix only the change in pressure. For a unique solution, you must also specify a reference pressure. In this example, the pressure at the point (0,0) is fixed. With the Darcy's Law interface, you express all these conditions as

$$\begin{array}{lll} \mathbf{n} \cdot \rho\mathbf{u} = 0 & \partial\Omega & \text{Sides} \\ p = p_0 & \partial^2\Omega & \text{Point} \\ p(x, y, 0) = \rho_0 g D & t = 0 & \text{Initial value} \end{array}$$

where $\mathbf{n}$ is the unit vector normal to the boundary, and p_0 is the reference pressure.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA

The governing equation for this problem is the conservative form of the Transport of Diluted Species in Porous Media interface

$$\frac{\partial \theta_s c}{\partial t} + \mathbf{u} \cdot \nabla c - \nabla \cdot \theta_s \tau D_L \nabla c = 0$$

where D_L is the fluid's diffusion coefficient (m^2/d); θ_s is the fluid's volume fraction (porosity); c is the salt concentration (mol/m^3), and $\mathbf{u}$ is the Darcy velocity (m/s).

In Elder's problem, the contaminant spreads only by advection and molecular diffusion, and the salt concentration is normalized to unit values.

The only contaminant source in the model domain is the salt concentration along the right half of the upper boundary. The vertical edge at $x = 300$ m is a symmetry boundary. The remaining boundaries have zero flux. The initial concentration is zero. The following equations represent these conditions:

$$\begin{array}{lll} \mathbf{n} \cdot [c\mathbf{u} - \theta_s \tau D_L \nabla c] = 0 & \partial\Omega & \text{Sides} \\ c = c_s & \partial\Omega & \text{Salt} \\ c(x, y, 0) = 0 & t = 0 & \text{Initial value} \end{array}$$

where $\mathbf{n}$ is the unit vector normal to the boundary.

Model Data

The example works with the following data:

PARAMETER	NAME	VALUE
ρ_0	Fresh-water density	1000 kg/m^3
ρ_s	Salt-water density	1200 kg/m^3
κ	Permeability	0.5 Darcy
μ	Dynamic viscosity	0.001 Pa·s

PARAMETER	NAME	VALUE
g	Gravity	9.81 m/s^2
ε	Porosity	0.1
$\tau_L D_L$	Molecular diffusion rate	$3.56 \cdot 10^{-6}$ m^2/s
c_s	Salt-water concentration	1 mol/m^3
c_0	Fresh-water concentration	0 mol/m^3
β	Increase of water density due to concentration changes	200 kg/mol

Note that the original set of parameters for the Elder problem gives a global Peclet number equal to

$$\mathrm{Pe} = \frac{(\rho_s - \rho_0)g\kappa L}{\mu\varepsilon D_L} \sim 408$$

Here, the difference in water density is $\rho_s - \rho_0 = \beta(c_s - c_0) = 200\ \mathrm{kg/m^3}$, and the length scale L is 150 m. This high Peclet number poses extra difficulties to numerical schemes; see for instance (Ref. 5 to Ref. 7).

Results and Discussion

The following results come from the COMSOL Multiphysics solution to a benchmark buoyancy problem that is often used for both temperatures (Ref. 1) and concentrations (Ref. 2).

Figure 2 gives snapshots of concentrations at six times during the 20-year simulation period. Initially the water is pristine. By the end of the first year, concentrations spread by diffusion, creating a density gradient. The buoyancy flow begins at the edge of the salt contact, where there is a sharp contrast in fluid density. By the end of year three, the fingering of high concentrations into the reservoir is mature. By year 10, the salt concentrations have spread over roughly 60% of the model domain. The COMSOL Multiphysics solution in Figure 2 is in excellent agreement with that from Elder (Ref. 1).

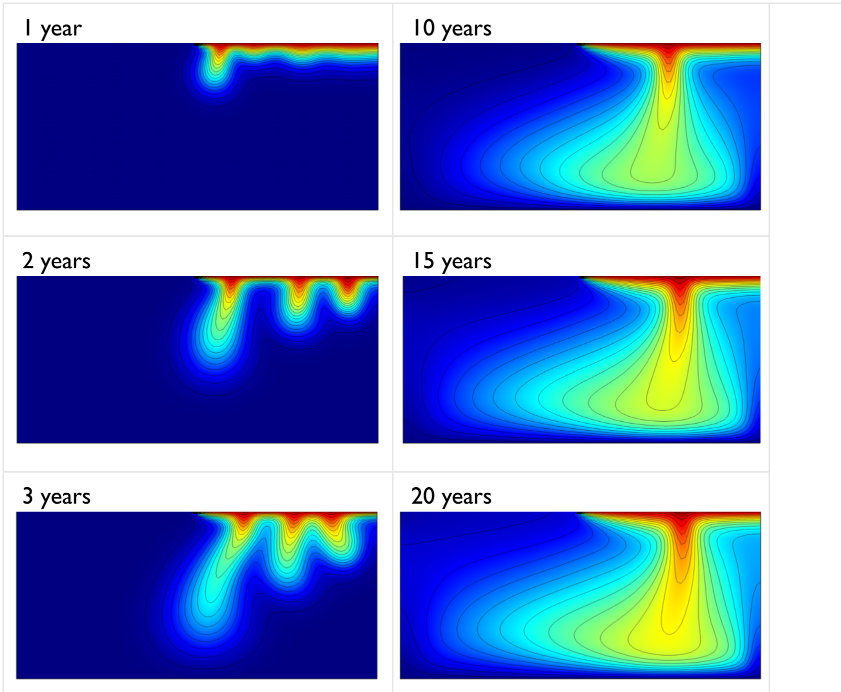

*Figure 2: Snapshots of concentrations from the COMSOL Multiphysics solution to the buoyancy-flow benchmark developed by Voss and Souza (*Ref. 2*) for the Elder problem.*

Figure 3 shows the concentration for the stationary Elder's problem.

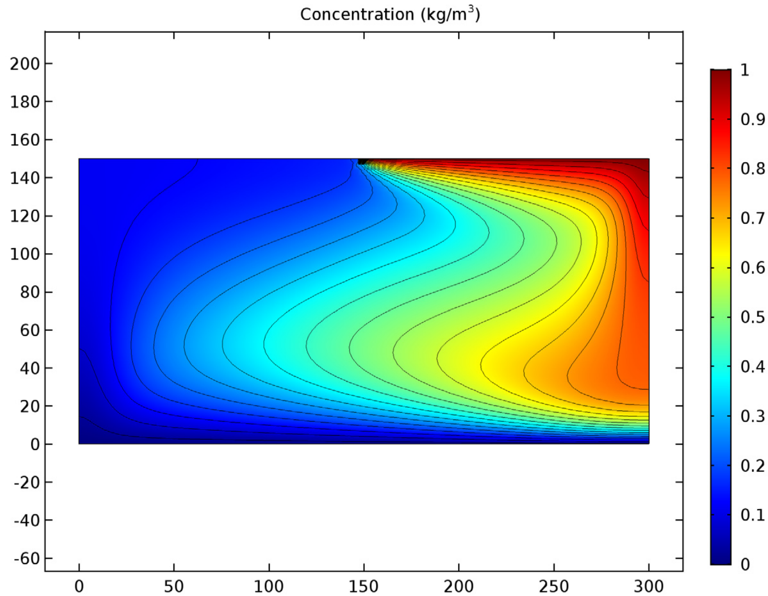

Figure 3: Concentration distribution from the COMSOL Multiphysics solution to the buoyancy-flow benchmark for the stationary Elder problem.

Of interest in the Elder problem is the development of convection cells. The COMSOL Multiphysics plots in Figure 4 reveal the convection cells with the help of velocity streamlines, which the figure shows simultaneously with concentrations for years 3, 10, 15, and 20. At early times, small convection cells develop between the individual fingers of the plume. At late times, a single convection cell covers the model domain.

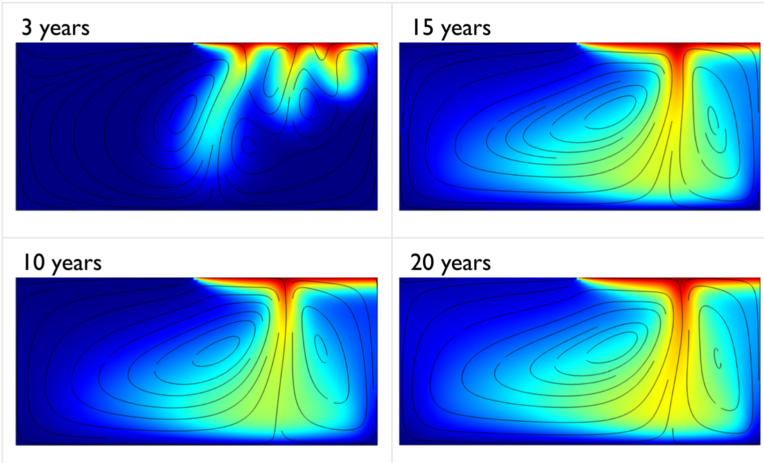

Figure 4: Salt concentrations (surface plot) and velocities (streamlines) from the COMSOL Multiphysics solution to a buoyancy benchmark problem (Ref. 2).

This example shows COMSOL Multiphysics applied to a well-known benchmark problem applicable to flow driven by density variations related to either temperature or concentration. The COMSOL Multiphysics results, here for concentration, closely match the benchmark solution (Ref. 2). This buoyant flow is straightforward to set up directly on top of a standard fluid flow and solute-transport model.

References

1. J.W. Elder, "Transient Convection in a Porous Medium," *J. Fluid Mechanics*, vol. 27, no. 3, 609–623, 1967.

2. C.I. Voss and W.R. Souza, "Variable Density Flow and Solute Transport Simulation of Regional Aquifers Containing a Narrow Freshwater-saltwater Transition Zone," *Water Resources Research*, vol. 23, no. 10, pp. 1851–1866, 1987.

3. C.I. Voss, "A Finite-element Simulation Model for Saturated-unsaturated, Fluid-density-dependent Ground-water Flow with Energy Transport or Chemically-reactive Single-species Solute Transport," *U.S. Geological Survey Water-Resources Investigation Report*, 84–4369, 1984.

4. W. Guo and C.D. Langevin, *User's Guide to SEAWAT: A Computer Program for Simulation of Three-Dimensional Variable-Density Ground-Water Flow*, U.S. Geological Survey Techniques of Water-Resources Investigations 6-A7, 2002.

5. P. Frolkovic and H. De Schepper, "Numerical modelling of convection dominated transport coupled with density driven flow in porous media," *Advances in Water Resources*, vol. 24, no. 1, pp. 63–72, 2000.

6. G.F. Carey, W. Barth, J. A. Woods, B. S. Kirk, M. L. Anderson, S. Chow, and W. Bangerth, "Modelling error and constitutive relations in simulation of flow and transport, " *Int. J. Numer. Meth. Fluids*, vol. 46, pp. 1211–1236, 2004.

7. J.A. Woods and G.F. Carey, "Upwelling and downwelling behavior in the Elder-Voss-Souza benchmark," *Water Resour. Res.*, vol. 43, W12403, 2007.

Application Library path: `Subsurface_Flow_Module/Solute_Transport/buoyancy_darcy_elder`

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 **Preset Studies for Selected Physics Interfaces>Time Dependent**.

8 Click **Done**.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
L	150[m]	150 m	Basin depth
rho0	1000[kg/m^3]	1000 kg/m³	Pristine water density
rho_s	1200[kg/m^3]	1200 kg/m³	Brine density
c0	0[mol/m^3]	0 mol/m³	Zero salt concentration
c_s	1[mol/m^3]	1 mol/m³	Normalized salt concentration
beta	(rho_s-rho0)/(c_s-c0)	200 kg/mol	Increase in density due to salt concentration
p0	0[atm]	0 Pa	Reference pressure
mu	1e-3[Pa*s]	0.001 Pa·s	Dynamic viscosity
kappa	500[mD]	4.9346E-13 m²	Permeability
epsilon	0.1	0.1	Porosity
D_L	3.56e-6[m^2/s]	3.56E-6 m²/s	Molecular diffusion
Pe	beta*(c_s-c0)*g_const*kappa*L/(mu*epsilon*D_L)	407.8	Peclet number

GEOMETRY 1

Rectangle 1 (r1)

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

2 In the **Settings** window for Rectangle, locate the **Size and Shape** section.

3 In the **Width** text field, type `2*L`.

4 In the **Height** text field, type `L`.

Point 1 (pt1)

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

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

3 In the **x** text field, type `L`.

4 In the **y** text field, type `L`.

5 Click **Build All Objects**.

DEFINITIONS

Add a variable for the buoyancy force due to concentration gradients.

Variables 1

1 On the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
rho	rho0+beta*c*(c>0)	kg/m³	Water density

DARCY'S LAW (DL)

Gravity 1

1 On the **Physics** toolbar, click **Domains** and choose **Gravity**.

2 In the **Settings** window for Gravity, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Gravity** section. From the **Specify** list, choose **Elevation**.

5 In the D text field, type `y-L`.

Fluid and Matrix Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law (dl)** click **Fluid and Matrix Properties 1**.

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

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

4 Locate the **Matrix Properties** section. From the κ list, choose **User defined**. In the associated text field, type `kappa`.

5 Locate the **Fluid Properties** section. From the μ list, choose **User defined**. In the associated text field, type `mu`.

6 Locate the **Matrix Properties** section. From the ε_p list, choose **User defined**. In the associated text field, type `epsilon`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law (dl)** click **Initial Values 1**.

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

3 In the p text field, type `p0+rho*g_const*dl.D`.

This defines the hydrostatic pressure distribution as reasonable initial condition.

Symmetry 1

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

2 Select Boundary 5 only.

3 In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.

Pointwise Constraint 1

1 On the **Physics** toolbar, click **Points** and choose **Pointwise Constraint**.

2 In the **Settings** window for Pointwise Constraint, locate the **Pointwise Constraint** section.

3 In the **Constraint expression** text field, type `p0-p`.

4 Select Point 2 only.

Since the pressure is not set explicitely by a boundary condition, you need to fix it at least at one point to get a unique solution for Darcy's Law.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Porous Media Transport Properties 1

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

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

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

4 Locate the **Diffusion** section. In the $D_{F,c}$ text field, type `D_L`.

5 From the **Effective diffusivity model** list, choose **Tortuosity model**.

6 In the $\tau_{F,c}$ text field, type `1`.

7 Locate the **Model Inputs** section. From the $\mathbf{u}$ list, choose **Darcy's velocity field (dl)**.

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 `c0`.

4 In the **Model Builder** window, click **Transport of Diluted Species in Porous Media (tds)**.

Symmetry 1

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

2 Select Boundary 5 only.

Concentration 1

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

2 Select Boundary 2 only.

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

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

5 In the $c_{0,c}$ text field, type `c0`.

Concentration 2

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

2 Select Boundary 4 only.

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

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

5 In the $c_{0,c}$ text field, type `c_s`.

MESH 1

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

Size

1 In the **Settings** window for Size, locate the **Element Size** section.

2 From the **Predefined** list, choose **Extremely fine**.

3 Click **Build All**.

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 **a**.

3 In the **Times** text field, type `range(0,1,20)`.

4 On the **Home** toolbar, click **Compute**.

RESULTS

Pressure (dl)

1 Click the **Zoom Extents** button on the **Graphics** toolbar.

The first default plot group shows the pressure distribution due to gravity.

Concentration (tds)

The second default plot group shows the concentration after 20 years. To reproduce the series of plots in Figure 2, add a Contour node and plot for different times.

Contour 1

1 In the **Model Builder** window, under **Results** right-click **Concentration (tds)** 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 **Model>Component 1>Transport of Diluted Species in Porous Media>c - Concentration**.

3 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

4 From the **Coloring** list, choose **Uniform**.

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

Concentration (tds)

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

2 In the **Settings** window for 2D Plot Group, click to expand the **Title** section.

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type Concentration (kg/m³).

5 Click to collapse the **Title** section. On the **Concentration (tds)** toolbar, click **Plot**.

6 Locate the **Data** section. From the **Time (a)** list, choose **1**.

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

Compare the result with the upper-left plot in Figure 2.

Repeat the previous two steps for the Time values 2 years, 3 years, 10 years,15 years, and 20 years to reproduce the remaining five plots in the series.

To reproduce the combined concentration/velocity plots in Figure 4, proceed as follows.

8 Right-click **Results>Concentration (tds)** and choose **Duplicate**.

Contour 1

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

Concentration (tds) 1

1. Right-click **Contour 1** and choose **Delete**.

   Click **Yes** to confirm.

Streamline 1

1. In the **Model Builder** window, under **Results** right-click **Concentration (tds) 1** and choose **Streamline**.
2. In the **Settings** window for Streamline, locate the **Streamline Positioning** section.
3. From the **Positioning** list, choose **Uniform density**.

Concentration (tds) 1

1. In the **Model Builder** window, under **Results** click **Concentration (tds) 1**.
2. In the **Settings** window for 2D Plot Group, locate the **Data** section.
3. From the **Time (a)** list, choose **3**.
4. Click to expand the **Title** section. In the **Title** text area, type Surface: Concentration (kg/m³)   Streamlines: Velocity field.
5. Click to collapse the **Title** section. On the **Concentration (tds) 1** toolbar, click **Plot**.

   Compare the result with the upper-left plot in Figure 4.

   Repeat the previous two steps for the Time values 10 years, 15 years, 20 years to reproduce the remaining three plots in the series.

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>Stationary**.
4. Click **Add Study** in the window toolbar.
5. On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

1. In the **Model Builder** window, click **Study 2**.
2. In the **Settings** window for Study, locate the **Study Settings** section.
3. Clear the **Generate default plots** check box.
4. On the **Home** toolbar, click **Compute**.

RESULTS

To visualize the stationary concentration distribution, use the second plot group as the starting point.

Concentration (tds)

In the **Model Builder** window, under **Results** right-click **Concentration (tds)** and choose **Duplicate**.

Concentration (tds) 2

1 In the **Settings** window for 2D Plot Group, locate the **Data** section.
2 From the **Data set** list, choose **Study 2/Solution 2 (sol2)**.
3 On the **Concentration (tds) 2** toolbar, click **Plot**.
4 Click the **Zoom Extents** button on the **Graphics** toolbar.

   Compare the resulting plot with that in Figure 3.