

Buoyancy Flow with Darcy's Law — The Elder Problem

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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 (Ref. 8) 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 by coupling two physics interfaces: Darcy's Law and Transport of Diluted Species in Porous Media.



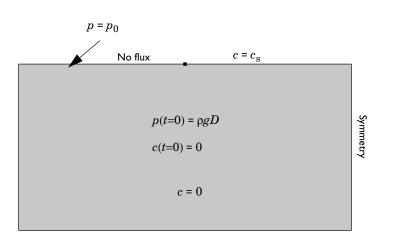


Figure 1: Geometry for modeling the Elder problem with initial conditions and boundary conditions indicated. In this cross section of a water-saturated porous medium, high salt concentrations exist in the top-right region.

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:

$$\frac{\partial \varepsilon_{p} \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$
$$\mathbf{u} = -\frac{\kappa}{\mu} (\nabla p + \rho g \nabla D)$$

Here, ρ is the water density (kg/m³), *t* is the time (s), $\varepsilon_{\rm p}$ is the porosity, and **u** is the vector of directional seepage rates, also known as the Darcy velocity. The Darcy velocity **u** depends on the permeability κ (m²), the fluid's dynamic viscosity μ (Pa·s), the fluid's pressure *p* (Pa), and the acceleration of gravity *g* (m/s²). 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, $c \pmod{m^3}$ 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

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

where **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

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

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/m³), and **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:

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

where **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
$\rho_{\rm s}$	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	
3	Porosity	0.1	
$\tau_L D_L$	Molecular diffusion rate	3.56·10 ⁻⁶ m ² /s	
$c_{\rm s}$	Salt-water concentration	I 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

$$Pe = \frac{(\rho_{\rm s} - \rho_0)g\kappa L}{\mu \varepsilon_{\rm p} D_L} \sim 408$$

Here, the difference in water density is $\rho_s - \rho_0 = \beta(c_s - c_0) = 200 \text{ kg/m}^3$, 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).

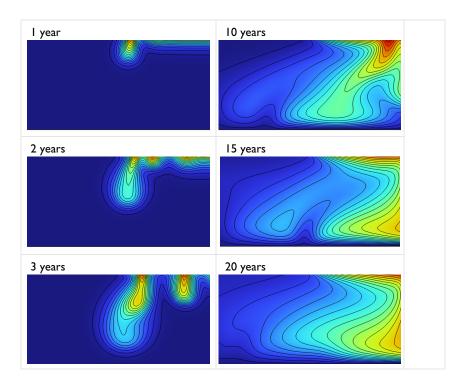


Figure 2: Snapshots of concentrations from the COMSOL Multiphysics solution to the buoyancy-flow benchmark developed by Voss and Souza (Ref. 2) for the Elder problem.

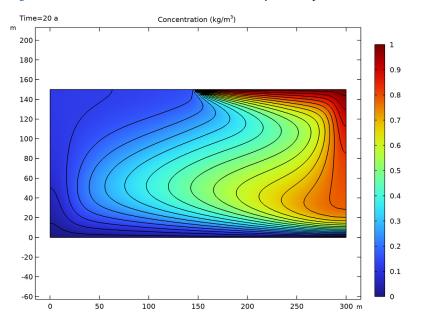


Figure 3 shows the concentration for the stationary Elder's problem.

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.

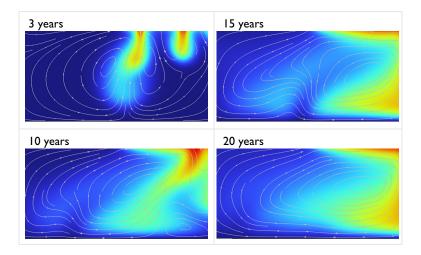


Figure 4: Salt concentrations (surface plot) and velocities (streamlines) from the COMSOL Multiphysics solution to a buoyancy benchmark problem (Ref. 2).

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, pp. 609–623, 1967.

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3. C.I. Voss, "A Finite-element Simulation Model for Saturated-unsaturated, Fluiddensity-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.

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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.

8. J. W. Elder et al "The Elder Problem", Fluids, vol. 2, p. 11, 2017.

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

- I In the Model Wizard window, click 9 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>Time Dependent.

8 Click **M** Done.

GLOBAL DEFINITIONS

Start by loading parameters from a file.

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** Click **b** Load from File.
- 4 Browse to the model's Application Libraries folder and double-click the file buoyancy_darcy_elder_parameters.txt.

GEOMETRY I

Rectangle 1 (r1)

- I 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 2*L.
- 4 In the **Height** text field, type L.

Point I (ptl)

- I In the **Geometry** toolbar, click **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 I

- I In the Home toolbar, click $\partial =$ 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	rhoO+beta*c*(c>O)	kg/m³	Water density

DARCY'S LAW (DL)

- I In the Model Builder window, under Component I (compl) click Darcy's Law (dl).
- 2 In the Settings window for Darcy's Law, locate the Gravity Effects section.
- 3 Select the Include gravity check box.

Gravity I

- I In the Model Builder window, under Component I (compl)>Darcy's Law (dl) click Gravity I.
- 2 In the Settings window for Gravity, locate the Gravity section.
- **3** From the **Specify** list, choose **Elevation**.
- 4 Select the Specify reference position check box.
- **5** Specify the \mathbf{r}_{ref} vector as

0 x

Ly

Fluid I

- I In the Model Builder window, under Component I (compl)>Darcy's Law (dl)> Porous Medium I click Fluid I.
- 2 In the Settings window for Fluid, locate the Fluid Properties section.
- **3** From the ρ list, choose **User defined**. In the associated text field, type rho.
- 4 From the μ list, choose User defined. In the associated text field, type mu.

Porous Matrix I

- I In the Model Builder window, click Porous Matrix I.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- ${\bf 3}\;$ From the ϵ_p list, choose ${\bf User}\; {\bf defined}.$ In the associated text field, type ${\tt epsilon}.$
- **4** From the κ list, choose **User defined**. In the associated text field, type kappa.

Initial Values 1

- I In the Model Builder window, under Component I (compl)>Darcy's Law (dl) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** Click the **Hydraulic head** button.

With gravity active, an initial zero hydraulic head defines the hydrostatic pressure distribution as reasonable initial condition.

Symmetry I

- I In the Physics toolbar, click Boundaries and choose Symmetry.
- 2 Select Boundary 5 only.
- **3** Click the **5** Show More Options button in the Model Builder toolbar.
- 4 In the Show More Options dialog box, in the tree, select the check box for the node Physics>Equation-Based Contributions.
- 5 Click OK.

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

Pointwise Constraint I

- I In 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.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Continue with setting up the species transport interface.

Fluid I

I In the Model Builder window, under Component I (compl)>

Transport of Diluted Species in Porous Media (tds)>Porous Medium I click Fluid I.

- 2 In the Settings window for Fluid, locate the Convection section.
- **3** From the **u** list, choose **Darcy's velocity field (dl/porous l)**.
- **4** Locate the **Diffusion** section. In the $D_{\text{F,c}}$ text field, type D_L.
- 5 From the Effective diffusivity model list, choose Tortuosity model.

Porous Matrix I

- I In the Model Builder window, click Porous Matrix I.
- 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 epsilon.

Initial Values 1

- I In the Model Builder window, under Component I (comp1)> Transport of Diluted Species in Porous Media (tds) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.

3 In the c text field, type c0.

Symmetry I

- I In the Physics toolbar, click Boundaries and choose Symmetry.
- **2** Select Boundary 5 only.

Concentration 1

- I In 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

- I In 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 I

Mapped I

In the Mesh toolbar, click Mapped.

Size

- I In the Model Builder window, click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 From the Predefined list, choose Extremely fine.
- 4 Click 📗 Build All.

STUDY I

Step 1: Time Dependent

- I In the Model Builder window, under Study I click Step I: Time Dependent.
- 2 In the Settings window for Time Dependent, locate the Study Settings section.
- 3 From the Time unit list, choose a.
- 4 In the **Output times** text field, type range(0,1,20).

It is a good idea to restrict the maximum time step size to capture the convective motion accurately.

Solution 1 (soll)

- I In the Study toolbar, click **Show Default Solver**.
- 2 In the Model Builder window, under Study I>Solver Configurations>Solution I (soll) click Time-Dependent Solver I.
- **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 Click **=** Compute.

RESULTS

Pressure (dl)

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 contours and plot for different times.

Contour I

- I In the Model Builder window, 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 Component I (compl)>

Transport of Diluted Species in Porous Media>Species c>c - Concentration - mol/m³.

- 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.

Streamline 1

In the Model Builder window, right-click Streamline I and choose Disable.

Concentration (tds)

- I In the Model Builder window, 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 Locate the Data section. From the Time (a) list, choose I.
- 6 In the Concentration (tds) toolbar, click 💽 Plot.

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

Repeat the previous two steps for 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.

Concentration (tds) 1

Right-click Concentration (tds) and choose Duplicate.

Contour I

- I In the Model Builder window, expand the Concentration (tds) I node.
- 2 Right-click Results>Concentration (tds) I>Contour I and choose Delete.
- 3 Click Yes to confirm.

Streamline 1

- I In the Model Builder window, under Results>Concentration (tds) I right-click Streamline I and choose Enable.
- 2 In the Settings window for Streamline, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>Darcy's Law> Velocity and pressure>dl.u,dl.v Darcy's velocity field.

Concentration and Velocity

- I In the Model Builder window, under Results click Concentration (tds) I.
- 2 In the Settings window for 2D Plot Group, type Concentration and Velocity in the Label text field.
- 3 Locate the Data section. From the Time (a) list, choose 3.
- 4 Locate the Title section. In the Title text area, type Surface: Concentration (kg/ m³) Streamlines: Velocity field.
- **5** In the **Concentration and Velocity** toolbar, click **I** Plot.

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

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

ADD STUDY

- I In the Home toolbar, click $\stackrel{\sim}{\sim}$ 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>Stationary.
- 4 Click Add Study in the window toolbar.
- 5 In the Home toolbar, click 2 Add Study to close the Add Study window.

STUDY 2

- I 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.

Step 1: Stationary

- I In the Model Builder window, under Study 2 click Step I: Stationary.
- **2** In the **Settings** window for **Stationary**, click to expand the **Values of Dependent Variables** section.
- **3** Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.
- 4 From the Method list, choose Solution.
- 5 From the Study list, choose Study I, Time Dependent.

The solution at the last time step is a good starting point for computing the stationary solution.

6 In the Home toolbar, click **=** Compute.

RESULTS

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

Concentration, Stationary

- I In the Model Builder window, right-click Concentration (tds) and choose Duplicate.
- 2 In the Settings window for 2D Plot Group, type Concentration, Stationary in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 2/Solution 2 (sol2).
- **4** In the **Concentration, Stationary** toolbar, click **O Plot**.

Compare the resulting plot with that in Figure 3.