

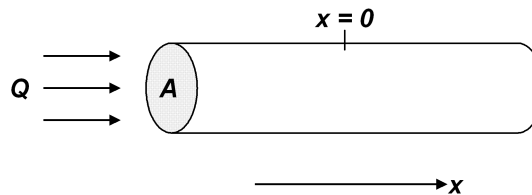
CGN 6933-002
Transport in Porous Media

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Homework #3
Due Fri., Feb. 11, 2005

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The purpose of this assignment is to begin developing an understanding of (1) the processes of advection, dispersion, and reaction, and (2) how these processes are represented in the advective-dispersive equation and its solutions.

Suppose you have a very long column filled with a porous medium – this could be, for instance, a reactor filled with catalyst beads, a column of activated carbon, a tube filled with sand, or something similar. You are pumping water through the column at a volumetric flow rate Q . The porosity of the medium is n . The cross-sectional area of the column is A . The longitudinal direction along the column (i.e., the direction of flow) is defined as the $+x$ -direction. See the figure below.



At time $t = 0$, a mass M of conservative tracer (e.g., bromide) is added very rapidly into the center of the column, which we shall designate $x = 0$. Suppose that you could inject the mass in such a way that it is distributed evenly across the cross-section of the column, but is added over a *negligible* thickness Δx in the direction of flow. In such a case, the initial concentration of the tracer in the column can be described by

$$C(x, t = 0) = \frac{M}{n A} \delta(x)$$

where C is the concentration of the tracer, and $\delta(x)$ is the Dirac function. For a conservative tracer, the transport through the porous medium can be described by the partial differential equation

$$n \frac{\partial C(x, t)}{\partial t} = n D \frac{\partial^2 C(x, t)}{\partial x^2} - n v \frac{\partial C(x, t)}{\partial x}$$

where D is the dispersion coefficient, and v is the water velocity through the column, which we can calculate from Q , A , and n .

If the column is long enough, then we can pretend it is infinitely long, in which case we can write the boundary conditions

$$C(x \rightarrow \pm\infty, t) = 0$$

So we have a partial differential equation with an initial condition and boundary conditions. The solution to the PDE with the given initial and boundary conditions is [see Kreft and Zuber, *Chem. Eng. Sci.*, 1978, vol. 33, pp. 1471-1480]:

$$C(x, t) = \frac{M}{n A} \frac{1}{\sqrt{4 \pi D t}} \exp \left[-\frac{(x - vt)^2}{4 D t} \right]$$

which gives us the concentration of the tracer in the column at any time and position.

- (1) Suppose that the column has a cross-sectional area $A = 50 \text{ cm}^2$, a velocity $v = 2 \text{ cm/d}$ (which would be realistic for groundwater flow), and a dispersion coefficient $D = 10 \text{ cm}^2/\text{d}$. The tracer mass added is $M = 1500 \text{ mg}$. The porosity is $n = 0.4$.
 - (a) Plot the concentration profile for the tracer (C vs. x) at time $t_1 = 50 \text{ d}$ and at time $t_2 = 200 \text{ d}$. Plot both profiles on the same graph. For each curve, determine C_{max} and the x -value at which C_{max} occurs. Hint: it is fine to do this problem in Excel, but in the long run, you will probably be happier if you do it in Matlab.
 - (b) For each curve, calculate the standard deviation of the spatial distribution, σ_x . On your curves, indicate (e.g., label by hand) the x values that correspond to distances of $\pm\sigma_x$ and $\pm 2\sigma_x$ from the peak location. Hint: if you are having trouble getting started on this part, then look up the equation for the probability density function (PDF) of the *normal distribution*, also called the Gaussian distribution or the “bell-shaped curve.” Does the PDF look familiar? (It should!) What is the standard deviation of the normal distribution? You can use that to help you find σ_x for our problem here.
 - (c) How does the elapsed time affect the peak concentration, C_{max} ? How does the elapsed time affect the location of the peak? How does the elapsed time affect the spread of the concentration distribution, L_x ? (There are different ways to define L_x ; one good way would be to say that L_x is the range of x for which $C > 0.01C_{max}$).

Now suppose that, instead of the conservative tracer that you considered above, you injected a soluble form of Strontium 89 (^{89}Sr), which undergoes radioactive first-order decay. The half-life of ^{89}Sr is about 50 days, which means it has a first-order decay constant $k = 0.014 \text{ d}^{-1}$. Then the transport equation needs to be modified to the following:

$$n \frac{\partial C(x, t)}{\partial t} = n D \frac{\partial^2 C(x, t)}{\partial x^2} - n v \frac{\partial C(x, t)}{\partial x} - n k C(x, t)$$

which has the following solution for the given initial and boundary conditions.

$$C(x, t) = \frac{M}{n A} \frac{1}{\sqrt{4 \pi D t}} \exp \left[-\frac{(x - vt)^2}{4 D t} \right] \exp (-k t)$$

- (2) Suppose that you inject 1500 mg of soluble ^{89}Sr instead of 1500 mg bromide. All other conditions are the same as in problem 1.
- For ^{89}Sr , again plot the concentration profile (C vs. x) for times $t_1 = 50 \text{ d}$ and $t_2 = 200 \text{ d}$. Compare to the conservative tracer. How does the first-order decay affect the peak concentration, C_{max} ? How does the first-order decay affect the spread of the concentration distribution, L_x ?
 - What fraction of the original mass remains at time $t_1 = 50 \text{ d}$? What fraction remains at time $t_2 = 200 \text{ d}$? How would these results be different if the ^{89}Sr were put into a plug-flow reactor, i.e., into a reactor with no dispersion? How would the results be different if the ^{89}Sr were put into a batch reactor, i.e., into a reactor with no flow? In other words, how does the mass remaining depend upon D and v ?

You might be thinking that these problems are not so realistic, because in reality, it is not possible to inject the mass over a *negligible* thickness Δx . You might be right; let's find out. Suppose that, instead, you injected the mass M of bromide or strontium over a time interval Δt_{pulse} . Then the concentration in the column is given by the following equation.

$$C(x, t) = \frac{1}{2} C_0 \left(\operatorname{erf} \left(\frac{0.5 v \Delta t_{pulse} - (x - v t)}{2 \sqrt{D t}} \right) + \operatorname{erf} \left(\frac{0.5 v \Delta t_{pulse} + (x - v t)}{2 \sqrt{D t}} \right) \right) \exp(-k t)$$

where C_0 is the initial concentration that results from the pulse addition, and erf is the error function.

- (3) Suppose that you injected 1500 mg of conservative tracer (e.g., bromide) over a time period $-7.5 \text{ d} < t < 7.5 \text{ d}$, i.e., $\Delta t_{pulse} = 15 \text{ d}$.
- What is the initial concentration, C_0 , of tracer that results from the pulse addition?
 - Plot the spatial distribution of the tracer (i.e., C vs. x) for the times $t_1 = 50 \text{ d}$ and $t_2 = 200 \text{ d}$.
Hint: Excel doesn't handle error functions very well, so you might want to try MatLab. Compare the peak heights and the spreads to those that you calculated in problem 1.
 - Discuss briefly the effect of the pulse form (infinitesimal vs. short duration) on the concentration distribution.
 - Do you think it is OK to use the idealized scenario given in problem 1, rather than the more realistic scenario given in problem 3? When might this idealization be OK? When would it not be OK? Explain.
- (4) Suppose that you injected 1500 mg of ^{89}Sr over a time period $-7.5 \text{ d} < t < 7.5 \text{ d}$, i.e., $\Delta t_{pulse} = 15 \text{ d}$. Plot the spatial distribution of the ^{89}Sr at times $t_1 = 50 \text{ d}$ and $t_2 = 200 \text{ d}$. Compare to the results you obtained at the same time in problem 2.
- (5) About how long (measured in hours) did it take you to complete this homework?