CGN 6933-002
Transport in Porous Media

Spring 2005 — University of South Florida
Homework #7 — Civil & Environmental Eng.
Due Fri., April 1, 2005 — J. A. Cunningham

Consider the transport of conservative bromide tracer through a column of porous medium. The transport can be described with the following partial differential equation.

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

Suppose that the column is initially devoid of any bromide mass, but that beginning at time $t = 0$, the bromide concentration at the front end of the column ($x = 0$) is held constant. The column has length L, and the back end of the column ($x = L$) is purged so that no bromide accumulates at that end. Then we can write the following initial and boundary conditions.

$$C(x, t = 0) = 0$$

$$C(x = 0, t \geq 0) = C_0$$

$$C(x = L, t) = 0$$

There is no analytical solution to the partial differential equation (PDE) with these initial and boundary conditions, so we will seek a numerical solution, as we did in the preceding homework assignment.

(1) In this problem, you will use a Crank-Nicolson method, and you will examine the effect of dispersion on numerical solutions.
   (a) Re-do part (a) of problem (2) from the previous homework assignment. This time use a Crank-Nicolson scheme. Use a time step $\Delta t = 0.05$ d. How do the profiles look compared to those in problems (2a) and (3a) from the previous homework assignment? Is there an obvious difference between the three methods?
   (b) Decrease the dispersion coefficient to $D = 0.33\ \mathrm{cm}^2/\mathrm{d}$. Re-run your program. Plot the results for $t = 1$ d and $t = 5$ d. Compare to the profiles from problem (1b) from the previous homework assignment. What happens to the numerical solution? Why? To facilitate your explanation, you might want to calculate the relevant Peclet numbers.

(2) We have looked at ways to use "finite differences" to approximate the spatial and time derivatives in the PDE. Typically we use "central-in-space" approximations for the spatial derivatives, because these approximations are second-order accurate. However, we could use an "upgradient" approximation, which is only first-order accurate, as follows.

$$\frac{\partial C(x,t)}{\partial x} \approx \frac{C(x,t) - C(x - \Delta x, t)}{\Delta x}$$

(a) Modify the Crank-Nicolson finite-difference code that you developed for problem (1). Use the upgradient approximation, as shown above, instead of the central-in-space derivative, for the *advective* term. Continue to use the central-in-space approximation for the dispersive term. This will probably require about a page of pencil-and-paper derivations before you are ready to modify your code. Hint: follow the same procedure that we developed in class, but just use this approximation for the spatial derivative instead. Turn in your new code. Put comments in your code as you think necessary or appropriate for me to follow it. Another hint: save your new code under a *new file name*, i.e., you do not want to erase or over-write your old code.

(b) Use your new "upgradient" code to plot the bromide concentration profiles at $t = 1$ day and $t = 5$ days. Use the following physical parameters: porosity $n = 0.30$, specific discharge $q = 1.5$ cm/d, dispersion coefficient $D = 0.33$ cm^2/d, and input concentration $C_0 = 100$ mg/L. Use the following numerical parameters: spatial discretization $\Delta x = 1$ cm, time step $\Delta t = 0.05$ d. Note that these are the same parameters you used for problem (1b) of this assignment.

(c) Compare your profiles from part (2b) to those you obtained in problem (1b). How do the profiles differ? What has been the effect of using the ugradient approximation instead of the central-in-space approximation?

(3) In this problem, your task is to figure out why the upgradient scheme from problem (2) has the effect that you saw. Proceed in the following manner. Re-run your program from problem (2), using different input values of D, until the profiles match those you generated in problem (1b). (Or, if you prefer, re-run your central-in-space code until the profiles match those from problem (2) – either way is fine.) Then, compare the values of D that result in matching profiles. The values of D differ by an amount that we will call Z. What value of Z do you find for the conditions of this problem? What does Z represent? Or, in other words, what does Z tell you about the upgradient approximation to the advective term?

(4) In this problem, your task is to come up with a general formula for Z, i.e., a formula that expresses Z in terms of known quantities. To do this, you will have to use the Taylor series for your approximations to the advective term. Develop one Taylor series for the central-in-space approximation, and develop another Taylor series for the upgradient approximation. Insert the Taylor series into the PDE, and compare the two; the difference between the two will enable you to determine the formula for Z. Does the value of Z that you found in problem (2) agree with the formula that you derived?

(5) About how long (measured in hours) did it take you to complete this homework?