CEE 557 **Spring 2016**

Due: Friday, April 1

Computer Problem #2

Part A - Finite Difference Methods

The purpose of this assignment is to analyze and compare numerical solutions to the 1D solute transport equation. This problem is divided into two parts: Part A covers finite difference methods; Part B covers finite element methods. You should work in teams, as in the first computer assignment.

The model problem is:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x}$$

$$c(x,0) = 0$$

$$\left(uc - D\frac{\partial c}{\partial x}\right)_{x=0} = uc_{Feed}\,,\ c_{Feed} = 1.0$$

$$c(x \to \infty, t) = 0$$

The analytical solution to this problem was discussed briefly in class. You can use the interactive applet to compute the solution; see: http://cee.uiuc.edu/transport, then go to "Equilibrium sorption with solute decay" and select "Third-Type BC." As we discussed in the class, you can use the interactive applet to evaluate the analytical solution, then copy and paste the results into another application (e.g. Excel, Matlab) for plotting and comparing with the numerical solution. If you prefer, you are free to write your own computer program to evaluate the analytical solution. In that case, you should consult the link "Summary of analytical solutions to nonreactive solute transport," that is listed on the course schedule on the compass site.

For this assignment, let u = 0.005 m/day. Think about how you will implement the flux boundary condition at x= 0, and the other boundary condition at x -> ∞

1. This first question considers explicit finite difference solutions; in particular, the upstream and central difference methods presented in class.
   (a) For $\Delta x = 0.05$ m, $\Delta t = 1$ day, $D = 2.5 \times 10^{-5}$ m^2/day, prepare amplitude ratio (AR) and phase error (PE) plots comparing the upstream and central difference methods. Include a table of results in an appendix. Also include a table showing AR and PE versus $\Lambda_n/\Delta x$. Discuss the differences between these two methods.

   (b) Use the upstream and central difference methods to solve equation (1) for the Δx, Δt, and D value given above. Plot the calculated concentration profiles at T = 50 days and 100 days, along with the analytical solution. Include a table of your results in an appendix. Discuss the behavior of the different solutions, particularly focusing upon numerical dispersion and oscillations. Are these results compatible with the information displayed in the Fourier Analysis of part (a)?

   (c) Choose the upstream method and calculate the solution using a Δt above the stability limit. Plot the solution to illustrate the behavior of an unstable method. What is the effect of the 3^{rd}-type boundary condition on the stability limit?

2. This question considers the Crank-Nicolson approximation to equation (1).

   (a) Generate amplitude ratio and phase error plots for the same parameters used in question 1(a). Discuss and compare your results.

   (b) Repeat question 1(b) using the Crank-Nicolson-Upwind and Central Methods. Discuss your results.

3. Evaluate the global mass balance for the numerical solutions in parts 1 and 2. You only need to perform the mass balance check on your numerical solution at T = 50 and 100 days. (That is, compare the total mass in the numerically computed profile with the theoretical value.) Include a table of your results. Discuss.

Extra Fun Problems (no points will be given, but could lead to ideas for a term project)

(a) In Q1 (b) above you should note that the upstream method is characterized by numerical dispersion and the central method is characterized by numerical oscillations. What would happen if you combined these methods by using: f*upwind + (1-f)*central, where $0<f<1$?

(b) Use the operator splitting approach described in class to solve this problem. For the advection term, use explicit upwind, and for the dispersion term use Crank-Nicholson. <u>Be careful</u> about the boundary conditions. In fact, you may want to formulate as a finite volume method instead of finite difference. Compare your results with those obtained in questions 1 and 2. Try a case where the time step is increased so that scriptU=1.0. Depending upon interest and time, also try a higher-order explicit method for the advection step.

Part B - Finite Element Methods for Solute Transport Problems

1. Use linear finite elements to solve the model 1D transport problem described in Part A. Write out the form of the element matrices and the system of global ODE's.

2. For $\Delta x = 0.05$m, $\Delta t = 1$ day, $D = 2.5 \times 10^{-5}$ m^2/day, $u = 0.005$m/day prepare AR and PE plots for Crank-Nicolson time stepping. Compare your results with those in Part A, Q2(a) for the finite difference method.

3. Use the Crank-Nicolson time stepping scheme to obtain an approximate solution. Plot the calculated concentration profiles at T = 50 days and T = 100 days, along with the analytical solution. Include a table of results. Perform a mass balance check on your numerical solutions. Compare the accuracy of this FE solution with the FD results of Part A, question 2(b). Which technique is more accurate? Is this consistent with the Fourier Analysis of AR and PE?

4. Evaluate the global mass balance for the FEM. Discuss.