Due 7 Dec 96

Objective: To understand various components and parameters in the solute mass transport equation.

Task: Your task is to run some FORTRAN solute transport models and compare the breakthrough curves for both (1) the different models assigned and (2) sensitivity of important parameters within the models. Your write-up should emphasize interpretation of the results. Values of input parameters (including ranges of values to try for sensitivity analysis) are up to you, but you should be able to defend your choices. You will also get to present your results to the class at our last meeting on 6 Dec.

Assigned Problems:

Name	Assigned Problem	Models
	Compare Solute Loading Functions	1,2,5,5a
	Compare Loading from vadose zone to loading from saturated zone	1,2,8,9
	Investigate solute decay and production	1,2,11,12
	Investigate sorption, including equilibrium and rate limited sorption.	2, 19a
	Compare 1-D and 3-D solutions	2,23

Notes: Model 5a is a pulsing source. Model 19a is the two-site sorption model; if F = 0 it becomes Model 19, and if F = 1 it becomes Model 20.

The written assignment may be done individually or with the other person working the same problem. The presentation in the class will be done with the other person who has also been assigned that problem.

The Models:

The models were developed by Dr. Kirk Hatfield from Univ. of Florida. They involve several steps:
1. Define the model governing equations and boundary conditions.
2. Transform these equations into Laplace space.
3. In Laplace space, the time variable disappears, and the equations can be solved analytically.
4. The Laplace solution is transformed back into real space.

The hand out does steps 1-3 for you. Step 4 is done numerically by a FORTRAN program. I have given you compiled models and sample input files that do step 4. You will get an ASCII file with the tabulated output data, which you can plot using EXCELL or MATHCAD or whatever.

Procedures:

- EDIT the input files (in*.dat) files to create the input parameters that you need. You can do this in NOTEPAD or any text editor. You can enter a range of time and space locations for the model to solve for resident concentrations. You do this by giving an initial time, a final time, and the number of times to be calculated. If you enter:

  0. 10. 11

  you will get solutions for t = {0,1,2,3,4,5,6,7,8,9,10}. Space parameters work the same way.
- Run the program (model*.exe) by typing the model name and pressing enter at the DOS prompt, or clicking on the file name in FILE MANAGER.
- The programs are set up to ask you the names (10 characters) of your input and output file as it runs. Import the data from output file (ASCII) into EXCELL or MATHCAD to plot.
- For the output filename, you need to make up a new file name that does not currently exist in your directory

Hints:

- Dr Hatfield used slightly different notation than what I use, in particular he uses "v" for Darcy flux.
- If you try to solve for t = 0, the program will bomb. I have tried to put in a "fail-safe" switch to solve for short times that are slightly greater than zero, but in doing so I assumed you would always be solving for more than one time step. Also, sometimes the programs will bomb when the concentration is too near zero. If the program bombs, try to adjust your input parameters to avoid solving for times/places where either t or C = 0.