CHE 581
Extra Credit: Assignment 7
**Due: 15 March 2019**

The convection-dispersion equation (CDE) is one that is used to describe the transport of chemical species in all kinds of media, including contaminant transport in rivers, groundwater, and the atmosphere.

For this problem, we want to look at reactive and non-reactive transport in a river. The CDE is given by

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

where $D$ is the effective dispersion coefficient, $v$ is the convective (fluid) velocity, and $k$ is the first-order decay coefficient.

Modify our code "impde.m" to solve the CDE for a river flow. Use $v$ = 1.2 km/hr, $D$ = 0.7 km$^2$/hr, with a total domain length of $L$ = 200 km (these values would be typical for the Willamette River, as reported in USGS Report 95-4078). For boundary conditions, use a a zero-derivative condition at both boundaries ($dc/dx = 0$ at $x = 0$ and $x = L$), and for the initial condition use a "hill" function (i.e., a Gaussian) of the form

$$f(x) = \exp[-0.1*(x - L/2)^2]$$

so that the initial condition is a pulse in the middle of our domain.

1. To solve this problem, first start by **creating a recurrence relationship** for the PDE using centered differences, and a Crank-Nicholson scheme (if you would like to try the theta method, please feel free to do so). Please show this work. Start by noting

   $$-v\frac{\partial c}{\partial x} = -v*\frac{1}{2}\left[\frac{c_{i+1}^{j+1} - c_{i-1}^{j+1}}{2\Delta x} + \frac{c_{i+1}^{j} - c_{i-1}^{j}}{2\Delta x}\right]$$

   and then carry out the computations illustrated in class (and in the code impde_2012) to find the implicit form of the equation. The result should look like (for the Crank-Nicholson method):

```
% ======================================================================
%
======================================================================
%      -(r+w)*c(i-1,j+1)+(2+2*r+kdt)*c(i,j+1)-(r-w)*c(i+1,j+1) =
%        (r+w)*c(i-1,j)+(2-2*r-kdt)*c(i,j)+(r-w)*c(i+1,j)
%
======================================================================
%
======================================================================
%
% where r = D*dt/(dx^2)
% kdt = k*dt
```

```
% w = v*dt/(2*dx)
```

2. Revise the code impde to reflect this problem statement.

3. Solve this problem for the **nonreactive** case for a time of $T = 60$ hours. Create a plot of the breakthrough curve (concentration versus time for a fixed spatial location) for the contaminant at location $x$=150 km. Use a time step of $\Delta t$=60/600, and a space step of $\Delta x$ = L/200

4. Solve this problem for the **reactive** case, with $k = 0.1$ hr$^{-1}$ over the same time interval and for the same breakthrough location. Compare the reactive and nonreactive solutions on the same plot. Use the same time and space steps as for the nonreactive case.

5. Do a "rough" convergence analysis on the nonreactive breakthrough curve. Do this by computing the solution using a number of spatial intervals equal to 40, 100, 200, and 500, and then plotting the results on the same graph. Do you see any difference in the solutions? If so, why do you think that this difference exists?

Complete a careful convergence analysis as follows. Starting with the $\Delta t$=60/150 and $\Delta x$ L/50 given above, solve the problem by successively cutting the time and space steps by a factor of 2. Do this 4 times (so that you will have five solutions total), i.e.

| | | |
|---|---|---|
| Case 1 | $\Delta t$=60/150 | $\Delta x$ L/50 |
| Case 2 | $\Delta t$=60/300 | $\Delta x$ L/100 |
| Case 3 | $\Delta t$=60/600 | $\Delta x$ L/200 |
| Case 4 | $\Delta t$=60/1200 | $\Delta x$ L/400 |
| Case 5 | $\Delta t$=60/2400 | $\Delta x$ L/800 |

To examine convergence, compute the following quantity for each successive set of simulations (i.e., 2, 3, 4, and 5)

$$\varepsilon_a(\text{case } i) = \frac{\displaystyle\int_{x=0}^{x=L}\int_{t=0}^{t=T} \left[c(x,t)\right]_{\text{resolutiomn } i} - \left[c(x,t)\right]_{\text{resolutiomn } i-1}\, dt\, dx}{\displaystyle\int_{x=0}^{x=L}\int_{t=0}^{t=T} \left[c(x,t)\right]_{\text{resolutiomn } i}\, dt\, dx} \times 100$$

And then plot this versus case number.