CHE 581
Assignment 6
Due: Wednesday, 13 March 2019
READ—Section 8.1 in Gerald and Wheatley (posted on Canvas)

24.8. (part b). Modify the code "bvp.m" to do this. In particular, code up the tridiagonal solver "Tridiag" given on page 247 and call that function to solve the system rather than relying on MATLAB's built-in solvers. Use only the finite difference method (part (b)).

24.11 Again, do this problem by modifying the code "bvp.m"; solve by calling the tridiagonal solver that you have coded up.

Additional Problems

(1) For the diffusion problem,

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

$$B.C.1 \quad \frac{\partial c}{\partial x} = 0 \quad \text{at } x = 0$$

$$B.C.2 \quad \frac{\partial c}{\partial x} = 0 \quad \text{at } x = L$$

$$I.C. \quad c = f(x) \quad \text{at } t = 0$$

Work out (using pencil and paper, or typed if you like...) the explicit finite-difference scheme that would apply to this problem. Show the set of equations for a 5-node system, and generate the arrays that would define the set of equations for any time step.

(2) Modify the code "xpde3.m" to do the following (using the initial condition already coded into the program):

(a) Compute the total mass in the system at each time step. The total mass is just the space integral of the concentration. Plot this as a function of time. Run the code for total time T=20 days, domain length L=0.1 m, and $\Delta x = L/40$ (or smaller!). Compute the total mass in the system as a function of time, and plot this (total system mass versus time). Does this plot correspond to your physical intuition of the system?

(b) Modify the code to account for a first-order reaction with rate coefficient, k, equal to 0.1 d^{-1}. this means that the equation that we need to solve is

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

$$B.C.1 \quad \frac{\partial c}{\partial x} = 0 \quad \text{at } x = 0$$

$$B.C.2 \quad \frac{\partial c}{\partial x} = 0 \quad \text{at } x = L$$

$$I.C. \quad c = f(x) \quad \text{at } t = 0$$

(c) Compute the total mass in the system as a function of time. Compare this with the total mass for the non-reactive case by preparing a plot showing both solutions as a function of time.