Project Statement:

The following differential equation describes the steady-state concentration of a substance that involves a first-order reaction in an plug-flow reactor tank (Figure 1):

$$D\frac{d^2c}{dx^2} - U\frac{dc}{dx} - kc = 0$$

where D=the dispersion coefficient [m^2/hr], c=the concentration [mol/L], x =distance [m], U=the mean velocity through the tank [m/hr], and k=the reaction rate [1/hr].

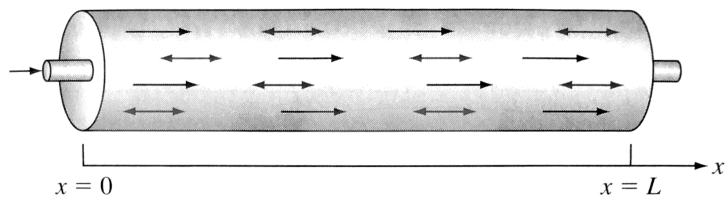

Figure 1. Schematic of an axially-dispersed plug-flow reactor tank.

The boundary conditions can be formulated as:

$$U\,c_{in} = Uc(x = 0) - D\frac{dc}{dx}(x = 0)$$

$$\frac{dc}{dx}(x = L) = 0$$

where c_{in} = the concentration in the inflow [mol/L] and L= the length of the reactor [m].

<u>Your solution and analysis should (at a minimum) focus on:</u>

i) Deriving the (centered) finite difference equations for this problem. [Hint: In particular make sure to use centered finite difference approximations of the same accuracy in the governing equation and the boundary conditions. The derivative boundary conditions will yield concentrations at ghost nodes that can be eliminated similarly to as shown in lecture notes.]

ii) Developing a solver code to solve the governing equation (which should itself be a function that can be called for a specified set of inputs).

iii) Using your solver to solve the governing equation for concentration as a function of distance given the following baseline parameters: D=5000 m^2/hr, U= 100 m/hr, and k=2/hr, L=100 m and c_{in}= 100 mol/L. Employ a spatial discretization of dx =5 m to obtain your solutions.

iv) Plotting the solution in terms of spatial distribution of c. In particular highlight the concentration leaving the tank under these parameters.

v) Exploring the impact of different design parameters (relative to the baseline) on the concentration leaving the tank. In particular, use your solver code to examine two additional cases (holding all other parameters equal to baseline values): 1) D=2500 m^2/hr and 2) U= 50 m/hr.