ChBE 2120, Numerical Methods
Homework 9

Paper and Pencil Portion

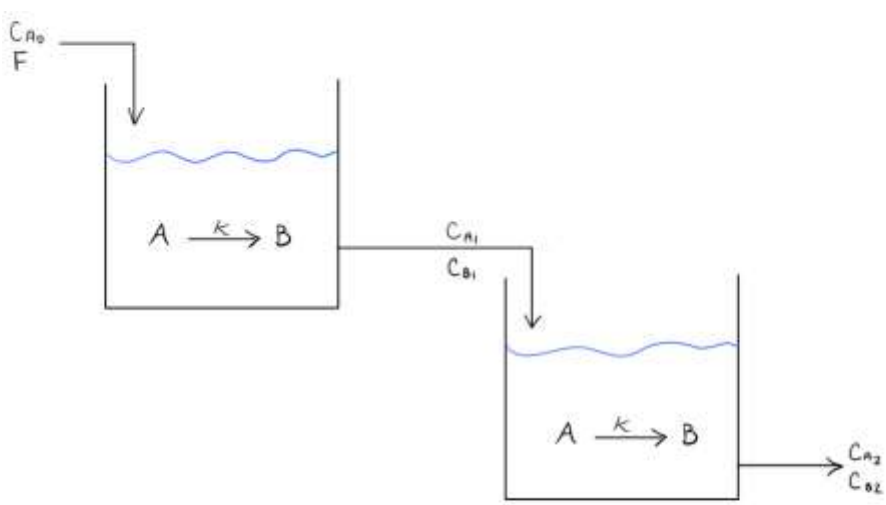
1) For Matlab Problem 1 below (textbook problem 28.8), you will use the method of Finite Differences to solve a differential equation. Show hand calculations to setup a matrix problem corresponding to the same problem and method. Use a step size Δx of 1 cm.

2) For Matlab Problem 2 below, (textbook problem 28.14), you will use the method of Finite Differences to solve a differential equation. Show hand calculations to setup a matrix problem corresponding to the same problem and method. Use a step size Δx of 20 m.

3) For this problem and Matlab problem 3 below, you will use the follow set up:

   A second-order irreversible reaction converts compound A to compound B in two stirred tank reactors at steady state. The tanks are fed with constant volumetric fluid flow rate. Each reactor contains a constant fluid volume, V. The reaction is characterized by a first-order rate constant, k.

   Stream Properties:
   F: volumetric flow rate for every stream
   $C_{A,0}$: concentration of A at the inlet of the first reactor
   $C_{A,1}$: concentration of A at the outlet of the first reactor
   $C_{A,2}$: concentration of A at the outlet of the second reactor
   $C_{B,1}$: concentration of B at the outlet of the first reactor
   $C_{B,2}$: concentration of B at the outlet of the second reactor



   a. Assume the following system of equations could be solved to determine the time dependences of the concentrations A and B in both reactors

$$\frac{dC_{A,1}}{dt} = \left(\frac{1}{\tau}\right)\left(C_{A,1} - C_{A,0}\right) - kC_{A,1}$$

$$\frac{dC_{B,1}}{dt} = -\left(\frac{1}{\tau}\right)\left(C_{B,1}\right) + kC_{A,1}$$

were τ equals $^{V}/_{F}$ and represents the "residence time" of fluid in each tank. Perform one iteration of the midpoint method to calculate the concentration of A and B at a time $\Delta\, t$ = 0.1 if $C_{A,0}$ = 10, $k = 0.5/min$ and $\tau = 6\ min$. The following initial conditions are

$$C_{A,1}|_{t=0} = 10$$
$$C_{B,1}|_{t=0} = 25$$

b. Now, assume the stirred-tank process is heated and a sudden change in heating rate results in the following equation for temperature in one of the tanks:

$$10\frac{d^2T}{dt^2} + 12\frac{dT}{dt} + T = 370$$

Put this differential equation into standard form by hand. Then, write a Matlab function that calculates, $\underline{f}$, a column vector first derivatives of the dependent variables for numerical (not functions of symbols) input values of t and Y. Note that $\underline{f}$ is used in the equations for initial value problem ODE solvers in your equation sheet (Euler's method, Midpoint method, Huen's method, Runge Kutta Methods).

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function [ f ] = TankTemperatureProfileFirstDerivative( t, Y)




end
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c. Set up the matrix equation for the Finite Differences approach to determine the tank's temperature profile for $0 \le t \le 10$ with a step size $\Delta t = 2$. Approximate derivatives using the lowest-order central finite difference formulas and use the following boundary conditions:

$$\frac{dT}{dt}|_{t=0} = 0$$

$$T|_{t=10} = 350K$$

MATLAB Portion

1) Problem 28.8 from the course textbook. Use a step size of 0.1cm and plot concentration of A as a function of distance

28.8 Compound A diffuses through a 4-cm-long tube and reacts as it diffuses. The equation governing diffusion with reaction is

$$D\frac{d^2A}{dx^2} - kA = 0$$

At one end of the tube, there is a large source of A at a concentration of 0.1 M. At the other end of the tube there is an adsorbent material that quickly absorbs any A, making the concentration 0 M. If $D = 1.5 \times 10^{-6}$ cm^2/s and $k = 5 \times 10^{-6}$ s^{-1}, what is the concentration of A as a function of distance in the tube?

2) Problem 28.14 from the course textbook. Use a step size of 1 m, although the textbook asks you to use a different step size. When calculating the values predicted by the analytical solution, use:

$$\lambda_1 = \frac{U}{2D}\left(1 - \sqrt{1 + \frac{4kD}{U^2}}\right), \lambda_2 = 1$$

28.14 The following differential equation describes the steady-state concentration of a substance that reacts with first-order kinetics in an axially-dispersed plug-flow reactor (Fig. P28.14),

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

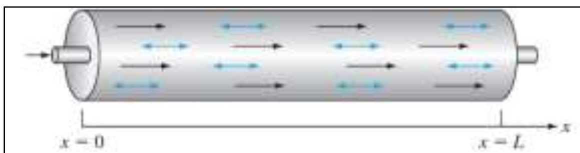

FIGURE P28.14
An axially-dispersed plug-flow reactor.

where D = the dispersion coefficient (m^2/hr), c = concentration (mol/L), x = distance (m), U = the velocity (m/hr), and k = the reaction rate (/hr). The boundary conditions can be formulated as

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

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

where c_{in} = the concentration in the inflow (mol/L), and L = the length of the reactor (m). These are called *Danckwerts boundary conditions*. Use the finite-difference approach to solve for concentration as a function of distance given the following parameters: $D = 5000$ m^2/hr, $U = 100$ m/hr, $k = 2$/hr, $L = 100$ m, and $c_{in} = 100$ mol/L. Employ centered finite-difference approximations with $\Delta x = 10$ m to obtain your solutions. Compare your numerical results with the analytical solution,

$$c = \frac{Uc_{in}}{(U - D\lambda_1)\lambda_2 e^{\lambda_2 L} - (U - D\lambda_2)\lambda_1 e^{\lambda_1 L}} \times (\lambda_2 e^{\lambda_2 L} e^{\lambda_1 x} - \lambda_1 e^{\lambda_1 L} e^{\lambda_2 x})$$

where

$$\frac{\lambda_1}{\lambda_2} = \frac{U}{2D}\left(1 \pm \sqrt{1 + \frac{4kD}{U^2}}\right)$$

3)

a. Solve the IVP in Paper and pencil 3a using Matlab. Integrate to $t = 10$ using Euler's method, midpoint method, RK4 and ode45 with $\Delta t = 0.1$. Plot all the results in one plot, and clearly label the plot.
b. Solve the BVP in Paper pencil 3c using Matlab. Find tank's temperature profile for $0 \leq t \leq 10$ with a step size $\Delta t = \mathbf{0.1}$. Plot the temperature profile you found.