Laboratory and Homework Assignment 8

Reading Assignment

1. "Chapter 8: Chemical Reactors" from Finlayson, Bruce A. Introduction to chemical engineering computing. John Wiley & Sons, 2012.

Laboratory Assignment (Due after laboratory session)

1. [30 points] Using Maltab, find the CSTR volume that achieves nearly 94% conversion of ethanol isothermally, for the following liquid-phase reaction. Assume the reactor is fed with 50 kgmol/h ethanol, 50 kgmol/h diethylamine, and 100 kgmol/h water. Following reaction takes place in the reactor:

$$A + B \rightarrow C + D, \tag{1}$$

where A=ethanol, B=diethylamine, C=water, and D=triethylamine. Assume rate of reaction is second order with respect to ethanol, i.e., $r_A = -kC_A^2$ and $k = A\exp(-E/RT)$. $E = 1 \times 10^4$ J/mol, $T = 50$°C, $A = 4775$ l/mol-h, $R = 8.314$ J/mol-K, $P = 3.5$ atm, molar density of ethanol is 17.132 mol/l; molar density of diethylamine is 9.678 mol/l; and molar density of water is 55.5 mol/l.

2. [30 points] Now using ASPEN and 'NRTL' as thermodynamic model, again solve the above problem. Note down the reactor volume you get from ASPEN in your answer-books. Do you get the same reactor volume; if no explain why?

3. Consider an ideal batch reactor. The tank is initially fed with 100 mol/m^3 of pure A and the mixture is left for 20 mins. A series chemical reaction takes place inside the tank

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \tag{2}$$

where k_1 and k_2 are the first order reaction rate constants. It is given that k_1 = 0.004 m^{3}mol^{-1} sec^{-1}. You are given that k_1/k_2 = 4.

   (a) [30 points] Apply component material balance to obtain differential equations in terms of C_A, C_B and C_C. Solve the differential equations either using ODE45 in Matlab or finite difference method. Plot the concentration of A, B and C as a function of time. Note the time at which the concentration of B is maximum. Justify your results using analytical solution. Also plot conversion of A vs overall yield of B.

   (b) [10 points] Now solve the differential equations for k_1/k_2 = 0.1, 1, 4, and 10. For these values of k_1/k_2, again plot the concentration of B as a function of time, and conversion of A vs overall yield of B. Are the results according to your expectations? If no, why?