CHG 3127
Assignment#4
(Due date: Assigned March 12/2011, Due March 22/2011)

Q1 (50%)

The reversible isomerization

$$A \rightleftharpoons B$$

is to be carried out in a membrane reactor (IMRCF). Owing the configuration of species B, it is able to diffuse out the walls of the membrane, while A cannot.

(a) What is the equilibrium conversion assuming that B does not diffuse out of the reactor walls?

(b) Plot the conversion profiles to compare a 100-dm^3 conventional PFR with a 100-dm^3 membrane reactor. What statements or generalizations can you make? What parameters have the greatest effect on the exit conversion shape of the plots in part (a)?

(c) Plot the conversion and the species concentrations and the molar flow rates down the length of the reactor.

Additional information:
Specific reaction rate = 0.05 s^{-1}
Transport coefficient k_c=0.3 s^{-1}
Equilibrium constant = K_e = 0.5
Entering volumetric flow rate υ_0 = 10 dm^3/s
C_{A0}=0.2 mol/dm^3

Q2 (50%)

The irreversible liquid phase acid catalyzed reaction

$$A \xrightarrow{H_2SO_4} C$$

is carried out in a semibatch reactor containing H_2SO_4. A is fed at a constant rate of 10 mol/min. The volumetric flow rate of liquid entering the semibatch reactor is 5 dm^3/min. The initial volume of a 3 M solution of H_2SO_4 catalyst in the reactor is 100 dm^3 (no A is present initially). The specific reaction rate is 0.05 min^{-1}. The reaction is first order in A and zero-order in catalyst concentration.

(a) Use POLYMATH or MATLAB to determine both the number of moles of A in the tank and the concentration of A and of H_2SO_4 as a function of time.
(b) Obtain an analytical solution for the number of moles of A, N_A , and the concentration of A, C_A, as a function of time. What is the concentration of A after 30 min? How many moles of A will there be in a tank after long times (i.e., $t \rightarrow \infty$)? (*Ans.:* N_A = 200 mol) Explain why the number of moles remains virtually constant at long times.

(c) Rework part (a) assuming the reaction is first order in H_2SO_4 with $k = 0.02$ $dm^3/$ mol · min.

(*Hint:* Do not try to use conversion in solving this problem!)