CE 561, Exam 2, December 15, 1999

This exam consists of four questions, each with multiple parts, and each worth 25% of the exam score. You should be careful not to get stuck on one part. If you do not know how to do a problem, move on and return to it if you have time at the end. If you cannot find the numerical answer to a problem, explain how you would find the answer if you had more time.
Carefully explain any assumptions you make, clearly indicate what part of what problem you are working on, and define the symbols that you use. The point value of each sub-part is indicated – budget your effort accordingly. There are 100 points total. Good luck.

1. The sequential first-order reactions

   A $\rightarrow$ B, with rate = $k_1 C_A$

   B $\rightarrow$ C, with rate = $k_2 C_B$

   are to be carried out in solution in a well-mixed isothermal batch reactor. Species B is the desired product, while species C is an undesired by-product. The values of the rate parameters are $k_1 = 0.3$ hr^{-1} and $k_2 = 0.6$ hr^{-1} at the operating temperature. At the start of each batch, the reactor is filled with a solution containing 2 moles of A per liter (and no B or C). The reactor volume is 500 liters. Emptying, cleaning, and re-filling the reactor between batches requires 15 minutes.
   (a) Find the **concentration of species B** in the reactor as a function of batch time. (10 pts.)
   (b) Find the **batch time** that maximizes the average production rate of species B. (10 pts.)
   (c) Find the **average production rate** of species B for this optimal batch time. (5 pts.)

2. The reversible, liquid phase, exothermic, first-order isomerization reaction

   A $\leftrightarrow$ B, with rate = $k_1 C_A - k_{-1} C_B$

   is to be carried out in a perfectly mixed adiabatic stirred tank reactor. Pure A is fed to the reactor. The rate parameters, reactor properties, and physical properties are as follows:

   Feed concentration of A = 8 moles/liter
   Feed temperature = 300 K
   Density of A = Density of B = 1.04 g/cm^3
   Specific Heat of A = Specific Heat of B = 2 J g^{-1} K^{-1}
   Heat of reaction = -41.6 kJ/mol
   Forward rate constant = $k_1 = 1\times10^8 \exp(-5000/T)$ hr^{-1}
   Reverse rate constant = $k_{-1} = 1\times10^5 \exp(-10000/T)$ hr^{-1}
   Feed flow rate = 100 liters hr^{-1}
   Reactor volume = 500 liters

   (a) Write the steady-state material and energy balances for this system and solve them to find the **steady-state temperature and composition** in the reactor. Be sure to solve for all possible steady states. (10 pts.)
   (b) Carry out a **linear stability analysis** for each set of steady-state operating conditions found in part (a) to show which are **stable** and which are **unstable**. (15 pts.)

3. Consider the dehydrogenation of ethylbenzene (EB) to styrene (S) in an adiabatic packed bed catalytic reactor

   EB $\leftrightarrow$ S + H_2

   Data for the reaction are as follows:

   Feed temperature = 925 K
   Feed pressure = 2.4 bar
   Molar flow of EB in the feed = 85 mol s^{-1}
   Molar flow of S in the feed = 0 mol s^{-1}
   Molar flow of H_2 in the feed = 0 mol s^{-1}
   Molar flow of H_2O in the feed = 1020 mol s^{-1} (H_2O does not react)
   Reaction rate = $k\,(p_{EB} - p_S p_{H2}/K)$ mol (kg catalyst)$^{-1}$ s^{-1}
   with $k = 3.46\times10^3 \exp(-10980/T)$ mol (kg catalyst)$^{-1}$ s^{-1} bar^{-1}
   and $K = 8.2\times10^6 \exp(-15200/T)$ bar
   (in the absence of any pore diffusion limitations)
   heat of reaction = -120 kJ mol^{-1}
   specific heat of feed mixture = 2.4 J g^{-1} K^{-1}
   molecular weight of EB = 106 g mol^{-1}

   (a) If the molar flow rate of styrene (S) at the reactor exit is 40 mol s^{-1}, what is the **temperature at the reactor exit**? (5 pts.)
   (b) Calculate the **mass of catalyst** required to achieve a styrene (S) molar flow rate of 40 mol s^{-1} at the reactor exit. (15 pts.)
   (c) Assuming the kinetics given above were measured in the absence of pore diffusion limitations, estimate the **maximum catalyst pellet diameter** for which pore diffusion limitations within the spherical catalyst pellets will be negligible throughout the reactor. Be sure to explain your reasoning. The catalyst density is 2.0 g cm^{-3}. The effective diffusion coefficient for EB in the catalyst pores is about 0.5 cm^2 s^{-1} in the temperature range in which the reactor is operated. (5 pts.)

4. The second order, irreversible reaction A + B $\rightarrow$ C + D to be carried out in an isothermal, partially mixed reactor. Tracer experiments show that the residence time distribution (RTD) for the reactor is well fit by the RTD for three equally-sized, perfectly-mixed tanks in series. The feed to the reactor is an equimolar mixture of A and B, with $C_{Ao} = C_{Bo}$ = 5 moles/liter. The mean residence time of the reactor is 10 minutes. The reaction rate is given by

   $r = 2\, C_A\, C_B$ mol liter^{-1} hr^{-1}, with C_A and C_B in moles per liter.

   (a) Derive the **dimensionless residence time distribution function** for three equally-sized perfectly-mixed tanks in series. (5 pts.)
   (b) Compute the **concentrations** of A and B in the reactor effluent using a **segregated flow** model with the RTD for 3 tanks in series. (8 pts.)
   (c) Compute the **concentrations** of A and B leaving the reactor by modeling the reactor as 3 perfectly-mixed **tanks in series** and solving species balance equations for the 3 tanks. (8 pts.)
   (d) **Explain any differences** between the results obtained in parts (b) and (c). (4 pts.)