CE 561, Exam 2, December 13, 2000

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 or computational resources. Note that a table of integrals is attached at the back of the test.

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.
Please use a separate blue book for each problem.
Good luck.

1. The autocatalytic reaction

   A + B $\rightarrow$ 2B, with rate = kC_AC_B

   is to be carried out in solution in a well-mixed isothermal batch reactor. The rate constant is 0.4 liter mol^{-1} hr^{-1} at the reaction temperature. At the start of each batch, the reactor is filled with a solution containing 2 moles of A per liter and 0.5 moles of B per liter. The reactor volume is 1000 liters. Emptying, cleaning, and re-filling the reactor between batches requires 1 hour.

   (a) Find the **concentrations of species A and 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 irreversible, liquid phase, exothermic, first-order isomerization reaction

   A $\rightarrow$ B, with rate = kC_A

   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 temperature = 300 K
   Density of A = Density of B = 1.04 g/cm^3
   Molecular Weight of A = Molecular Weight of B = 104 g/mol
   Specific Heat of A = Specific Heat of B = 2 J g^{-1} K^{-1}
   Heat of reaction = -41.6 kJ/mol
   Rate constant = $k = 1\times10^5 \exp(-5000/T)$ min^{-1}
   Feed flow rate = 100 liters min^{-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. The reversible, exothermic, first-order reaction A $\leftrightarrow$ B is to be carried out in aqueous solution at atmospheric pressure. At 300 K, the forward rate constant is 0.2 min^{-1} and the equilibrium constant is 1.0. The forward activation energy is 9.935 kcal/mol, and the heat of reaction is -10 kcal/mol. The properties of the solution can be assumed to be those of water (C_p = 1 cal g^{-1} K^{-1}, ρ = 1000 kg m^{-3}).
   (a) What is the maximum conversion of A to B that can be obtained in an adiabatic reactor with a feed temperature of 300 K and feed concentrations of C_{Ao} = 2.0 mol/liter, C_{Bo} = 0.0 mol/liter? (5 points)
   (b) What residence time is required to achieve 90% of the maximum conversion found in part (a) in an ideal CSTR with a feed temperature of 300 K and feed concentrations of C_{Ao} = 2.0 mol/liter, C_{Bo} = 0.0 mol/liter? (5 points)
   (c) What residence time is required to achieve 90% of the maximum conversion found in part (a) in an ideal PFTR with a feed temperature of 300 K and feed concentrations of C_{Ao} = 2.0 mol/liter, C_{Bo} = 0.0 mol/liter? (7 points)
   (d) For an adiabatic reactor with a feed temperature of 300 K C_{Bo} = 0.0 mol/liter, what is the maximum feed concentration of species A (C_{Ao}) for which the reactor contents will not boil no matter how long the residence time is? (8 points)

4. The second order, autocatalytic reaction A + B $\rightarrow$ 2 B 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 two perfectly-mixed tanks in series, with the first tank having a volume equal to twice that of the second tank. The feed to the reactor is a mixture of A and B, with C_{Ao} = 2 mol/liter and C_{Bo} = 0.5 mol/liter. The mean residence time of the reactor is 3 hours. The reaction rate is given by

   $r = 0.4\, C_A\, C_B$ mol $liter^{-1}$ hr^{-1}, with C_A and C_B in moles per liter.

   (a) Derive the **dimensionless residence time distribution function** for two perfectly-mixed tanks in series with the first tank having a volume equal to twice that of the second tank. (5 pts.)
   (b) Compute the **concentrations** of A and B in the reactor effluent using a **segregated flow** model with the RTD derived in part (a). (8 pts.)
   (c) Compute the **concentrations** of A and B leaving the reactor by modeling the reactor as 2 perfectly-mixed **tanks in series** and solving species balance equations for the 2 tanks. (8 pts.)
   (d) **Explain any differences** between the results obtained in parts (b) and (c). (4 pts.)

   Note that the reaction kinetics and feed concentrations are the same as in problem (1), so you may be able to re-use results derived there.