CE 561, Exam 2, December 9, 2008

This exam consists of three questions, each with multiple parts. 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. You may use three pages (2-sided) of hand-written notes.

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 = 1.0 hr^{-1} and k_2 = 1.5 hr^{-1} at the operating temperature. At the start of each batch, the reactor is filled with a solution containing 5 moles of A per liter (and no B or C). The reactor volume is 1000 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. (15 pts.)

   (c) Find the **average production rate** of species B for this optimal batch time. (5 pts.)

2. The irreversible, liquid phase, exothermic reaction

   A + B $\rightarrow$ C, with rate = $k_1 C_A C_B$

   is to be carried out in a perfectly mixed adiabatic stirred tank reactor. A solution containing equal amounts of A and B is fed to the reactor (mixing just prior to entering the reactor). The rate parameters, reactor properties, and physical properties are as follows:

   Feed concentration of A = Feed concentration of B = 10 mol/L

   Feed temperature = 300 K

   Density of feed = Density of product = 1.0 kg/L

   Specific Heat of feed = Specific Heat of product = 4.2 kJ kg^{-1} K^{-1}

   Heat of reaction = -42 kJ/mol

   Rate constant = $k_1 = 3\times10^{11}$ exp(-10000/T) L mol^{-1} hr^{-1}

   Feed flow rate = 100 liters hr^{-1}

   Reactor volume = 300 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. (15 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. (20 pts.)

3. Now, something a little different. Answer the following questions in a few sentences each:
   (a) Describe how, experimentally, you would determine whether internal diffusion limitations are important for a reaction being carried out using a high surface area porous heterogeneous catalyst. (5 points)
   (b) Explain how you would go about measuring an experimental residence time distribution for a reactor with an unknown degree of mixing. (5 points)
   (c) Write the balance equations for a single reaction in an adiabatic plug flow reactor with axial mixing, and explain how you would approach solving these equations. (5 points)
   (d) Write an equation for the pressure drop in a fixed-bed catalytic reactor, and explain how you would determine the parameter(s) that appear in the equation. (5 points)
   (e) Describe the first calculations you would make if you were assigned the task of designing a fixed-bed catalytic reactor for a new process. (5 points)
   (f) Explain why an inert diluent such as nitrogen might be added to the feed to a fixed bed reactor in which an exothermic reaction is taking place. (5 points)
   (g) Describe a situation in which it would be advantageous to use a batch reactor rather than a continuous reactor, and explain why it is advantageous. (5 points)