

CE 561, Exam 2, December 15, 2006

This exam consists of 3 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 or computational resources.

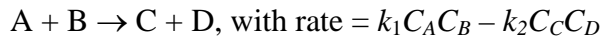
NOTE THAT ALL 3 PROBLEMS INVOLVE THE SAME REACTION

You may use a calculator and a single letter-size sheet (2-sided) of notes to aid you on this exam. You may not exchange notes with or otherwise consult your fellow students. If you talk to your fellow students during the exam, I will assume that you are cheating, you will be asked to leave, and you will fail the exam.

You will have 2 hours and 50 minutes to complete the exam. Please use a separate blue book for each exam problem. Carefully explain any assumptions you make, label what part of what problem you are working on, and define the symbols that you use. The point value of each part is indicated – budget your effort accordingly. There are 100 points total.

Good Luck!

1. The reversible, exothermic reaction



is to be carried out in solution in a well-mixed **adiabatic** batch reactor. At the start of each batch, the reactor contains 100 L of a solution of A and B at a concentration of 5 mol per liter ($C_{A0} = C_{B0} = 5$ mol/L) and a temperature of 300 K. Emptying, cleaning, and re-filling the reactor between batches requires 15 minutes. The reactor contents have a density of 1 kg per liter and a specific heat of 4200 J/(kg K). The forward and reverse rate constants are given by

$$k_1 = 5 \times 10^4 \exp(-5000/T) \quad \text{L}/(\text{mol min})$$

$$k_2 = 10^{11} \exp(-11000/T) \quad \text{L}/(\text{mol min})$$

where T is the temperature in Kelvins.

- Write the species mole balance and energy balance equations for the reactor and derive relationships that allow you to write the temperature and all species concentrations in terms of a single concentration or conversion variable. (10 pts.)
- Compute the maximum conversion of the reactants that can be obtained in this adiabatic batch reactor for the conditions given. (10 pts.)
- Compute the batch time required to convert 50% of the reactants to products. Even if you cannot evaluate this numerically, you should be able to write a single integral that, if evaluated, would give you the numerical answer. (10 pts.)
- Show, *in detail*, how you would find the batch time that maximizes the average production rate of the reaction products. You do not have to find the actual numerical solution. (10 pts.)

2. The same reaction described in problem 1 is to be carried out in a continuous, adiabatic perfectly mixed flow reactor (a CSTR). The reactor volume is 100 L, the feed stream contains 15 mol/L each of A and B and contains no C or D. The feed flow rate is 85 liters per minute. Other parameters are the same as in the previous problem.
- (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) Describe, in detail, how you would 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. You do not need to actually work out the numbers, but you should write out the equations. (10 pts.)
3. The same reaction treated in the previous two problems is 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 equally-sized, perfectly-mixed tanks in series. The total reactor volume is 200 L, the feed stream contains 1 mol/L each of A and B and contains no C or D. The feed flow rate is 100 liters per minute. The reactor temperature is 413.5 K, and at this temperature, $k_1 = k_2 = 0.280 \text{ L}/(\text{mol min})$.
- (a) Derive the dimensionless residence time distribution function for two equally-sized perfectly-mixed tanks in series. (10 pts.)
 - (b) Compute the concentrations of A and B in the reactor effluent using a segregated flow model with the RTD for 2 tanks in series. (10 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. (10 pts.)
 - (d) Explain any differences between the results obtained in parts (b) and (c). (5 pts.)