CE 561, Exam 2, December 11, 2003

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.

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 irreversible first order reaction

   A $\rightarrow$ B, with rate = kC_A with k = 0.2 hr^{-1}

   is to be carried out in aqueous solution in a well-mixed, isothermal, semi-batch reactor. At the start of each batch, the reactor is empty. It is then fed with a solution containing 2 moles of A per liter and no B. The feed flow rate is 500 liters per hour (this is the maximum allowable feed rate at which the reactor can be maintained isothermal). The reactor volume is 1000 liters, and when it is full, the feed is shut off. That is, the feed rate is 500 liters per hour for the first two hours, and 0 after the first two hours. Emptying and cleaning the reactor between batches requires 3 hours.

   (a) Find the **number of moles of species A and B** in the reactor as a function of time after the start of reactor filling (you should find solutions for all times, both before and after the feed is turned off). (15 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, exothermic, first-order isomerization reaction

   A $\rightarrow$ B, with rate = kC_A

   is to be carried out in aqueous solution in a perfectly mixed adiabatic stirred tank reactor. Properties of the reaction and reactor are as follows:

   Feed temperature = T_o = 300 K
   Feed Concentration of A = C_{Ao} = 1 mol/liter
   Heat of reaction = ΔH = -418,000 J/mol
   Density = ρ = 1000 g/liter
   Specific Heat = C_p = 4.18 J/(g K)
   Feed flow rate = Q = 50 liters min^{-1}
   Reactor volume = V = 100 liters

   The reaction rate constant can be expressed as

   $k = 10^{12} \exp(-10000/T)$ min^{-1}

(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. (15 pts.)

(3) Consider the production of SO_3 from SO_2 in a fixed bed tubular reactor. The overall reaction is $SO_2 + ½ O_2 \leftrightarrow SO_3$. The feed to the reactor is 0.5% by volume SO_2 and 99.5% by volume dry air (79% N_2, 21% O_2) at 450°C and 2 bar total pressure. The total feed flow rate is 500 kg/hr. The reactor will be a 50 cm diameter cylindrical vessel filled with catalyst pellets. The platinum on alumina catalyst is in the form of 4 mm diameter cylindrical pellets (ranging from 15 to 50 mm long), with a catalyst density of 1.0 g cm^{-3}, a pore volume of 0.4 cm^3 g^{-1}, and a specific surface area of 150 m^2 g^{-1}. The density of the catalyst bed, as packed in the reactor, is 0.6 (kg catalyst) m^{-3}. The pressure drop through the reactor is negligible. The reaction rate, in the absence of any diffusion limitations, is

$r = k_1 C_{SO_2} - k_2 C_{SO_3}$, with

$k_1 = 1.0\times10^6 e^{(-12000/T)}$ m^3 s^{-1} (kg catalyst)$^{-1}$ and $k_2 = 1.0\times10^{13} e^{(-24000/T)}$ m^3 s^{-1} (kg catalyst)$^{-1}$.

The specific heat of the gas mixture can be assumed constant at 1.0 kJ kg^{-1} K^{-1}. The atomic weights of sulfur, oxygen, and nitrogen are 32, 16, and 14 g mol^{-1}, respectively.

(a) Write the steady-state reactant (SO_2) mole balance equation and the enthalpy balance equation, including appropriate boundary conditions, for the fixed bed reactor for each of the following cases. Identify the variables in the equations and the units in which they are measured. Give their numerical values where possible. Where numerical values are not available from the problem statement, suggest how they might be obtained. For each part, give a <u>brief</u> description of how the balance equations could be solved numerically.

(i) Ideal plug flow, no radial or axial mixing, no heat flow through the reactor walls. (10 points)

(ii) Plug flow with mixing in the axial direction due to flow around the catalyst pellets, but still no heat flow through the reactor walls. (5 points)

(iii) Plug flow with both radial and axial mixing due to flow around the catalyst pellets and heat transfer through the reactor wall to condensing steam at 200 °C. (5 points)

(b) For *adiabatic operation* of the reactor with ideal plug flow and no radial or axial mixing, derive a relationship between the reactor temperature and the SO_2 conversion. Estimate the maximum temperature that could be reached in the reactor. What are the concentrations of SO_2 and SO_3 when this maximum temperature is reached? (10 points)

(c) Assuming there are no diffusional limitations, estimate the amount of catalyst and the reactor length (catalyst bed depth) required to achieve 80% of the maximum possible conversion of SO_2 to SO_3 in this reactor. (10 points)