

CE 561, Exam 2, December 10, 2007

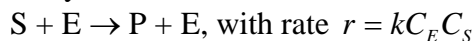
This exam consists of 3 questions, each with multiple parts. You should be careful not to get stuck on one part. If you do not know how to do a problem, move on and return to it if you have time at the end. If you cannot find the numerical answer to a problem, explain how you would find the answer if you had more time or computational resources.

You may use a calculator and up to three letter-size sheets (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 3 hours 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.

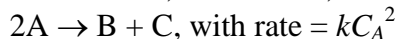
1. The enzymatic reaction



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 per liter of the substrate S and 0.05 moles per liter of the enzyme E. The feed flow rate is 50 liters per hour. The reactor volume is 100 liters, and when it is full, the feed is shut off. That is, the feed rate is 50 liters per hour for the first two hours, and 0 after the first two hours. Emptying and cleaning the reactor between batches requires 1 hour. The rate constant is $k = 5$ liter/(mol hr).

- Find the **number of moles of substrate (S) and product (P)** 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.)
- Find the **batch time** that maximizes the average production rate of product (P). (15 pts.)
- Find the **average production rate** of product (P) for this optimal batch time. (5 pts.)

2. The irreversible, exothermic, second-order reaction



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

Feed temperature = $T_o = 290$ K

Feed Concentration of A = $C_{Ao} = 2$ mol/liter

Heat of reaction = $\Delta H = -83600$ J/mol

Density = $\rho = 1000$ g/liter

Specific Heat = $C_p = 4.18$ J/(g K)

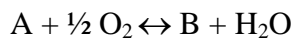
Feed flow rate = $Q = 20$ liters min^{-1}

Reactor volume = $V = 200$ liters

The reaction rate constant is given by

$$k = 5 \times 10^{25} \exp(-19000/T)$$

- (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. (18 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**. (18 pts.)
3. Consider the oxidative dehydrogenation of A to B in an adiabatic packed bed catalytic reactor:



Data for the reaction are as follows:

Feed temperature = 500 K

Feed pressure = 4 bar

Molar flow of A in the feed = 50 mol s⁻¹

Molar flow of O₂ in the feed = 500 mol s⁻¹

Molar flow of B in the feed = 0 mol s⁻¹

Molar flow of H₂O in the feed = 1000 mol s⁻¹

Reaction rate = $k (p_A p_{O_2}^{0.5} - p_B p_{H_2O}/K)$ mol (g catalyst)⁻¹ s⁻¹
with $k = 10^{13} \exp(-10000/T)$ mol (g catalyst)⁻¹ s⁻¹ bar^{-1.5}
(in the absence of any pore diffusion limitations)
and $K = 10^{12} \exp(-12000/T)$ bar^{0.5}

heat of reaction = -100 kJ mol⁻¹

specific heat of feed mixture = 2.0 J g⁻¹ K⁻¹

molecular weight of A = 100 g mol⁻¹

- (a) If the molar flow rate of B at the reactor exit is 30 mol s⁻¹, what is the **temperature at the reactor exit**? (5 pts.)
- (b) Calculate the **mass of catalyst** required to achieve a molar flow rate of B of 30 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 A in the catalyst pores is about 0.1 cm² s⁻¹ in the temperature range in which the reactor is operated. (9 pts.)