Chemical & Biomolecular Engineering 142

Chemical Kinetics and Reaction Engineering

Midterm 1

Tuesday, October 4, 2011

The exam is 100 points total and 20% of the course grade. Please read through the questions very carefully before answering. Make sure to show all your work. Good luck !

Name ___________________ _______________________________

Student ID____

Problems	Points (Max.)	Points Received
1		
2		
3		
4		
5		

You are allowed one 8.5”’x 11” sheet of paper and a calculator for this exam. A list of (possibly) useful integrals and constants is provided on the last page of this exam.

Problem 1

Your firm's trademark chemical is produced in an isothermal gas-phase batch reactor:

$$A + 2B \rightarrow P$$

The proposed elementary steps are

Rates	Steps	σ
r_1, r_{-1}	$A \leftrightarrow 2I^*$	
r_2	$I^* + B \rightarrow B^*$	
r_3	$2B^* \rightarrow P$	

(a) Fill in the σ's in the table above.
(b) Derive the rate expression using PSSH (pseudo-steady state hypothesis) alone.
(c) According to PSSH, what must be the relative rates of steps 1-3 above? In other words, how is r_1 related to r_{-1}, r_2 and r_3.
(d) Now apply QE (quasi-equilibrium) on the first step and derive the rate expression.
(e) By comparing (b) and (d), provide the rigorous justification for QE in this system.
(f) Draw the rate arrow diagram for the reaction sequence if QE is valid and clearly label the rates being graphed.
(g) Draw the rate arrow diagram for the reaction sequence if step 1 is practically irreversible.
(h) Given that QE is valid, what is the conversion of your reaction after 3.16 hours? (Note that $3.16 \sim \sqrt{10}$). The reactor is loaded with stoichiometric amounts of A and B at t=0 and c_{A0}=0.005M.

Rate Constant	k_1	k_{-1}	k_2	k_3
Values	16 h^{-1}	1 M^{-1} h^{-1}	5 M^{-1} h^{-1}	200 M^{-1} h^{-1}

Problem 2

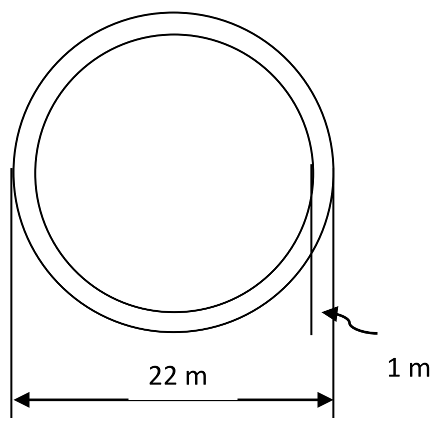
The gas phase (ideal gases) reaction,

$$3A + B \rightarrow 2C + D$$

A constant-volume batch reactor is a cylinder that is 22 meters in outer diameter and the outer metal wall is 1 meters thick. It measures 10 meters in height. The outside of reactor is exposed to atmosphere. It is initially filled with stoichiometric amounts of gaseous A and B, for a total amount of 150000 mols initially in the reactor. The reaction is started at t=0 with the rate law being

$$r = kc_A^2 c_B^{0.5}$$

with k=0.3 $M^{-1.5}$ day^{-1} at room temperature.



The container can withstand a maximum gauge pressure of 0.20 atm (both +0.20 atm and -0.20 atm). When will the reactor implode, if at all, upon itself? Report both the time and the conversion of the reactor at the time of implosion if it happens.

1 atm = 101325 Pascals

Problem 3

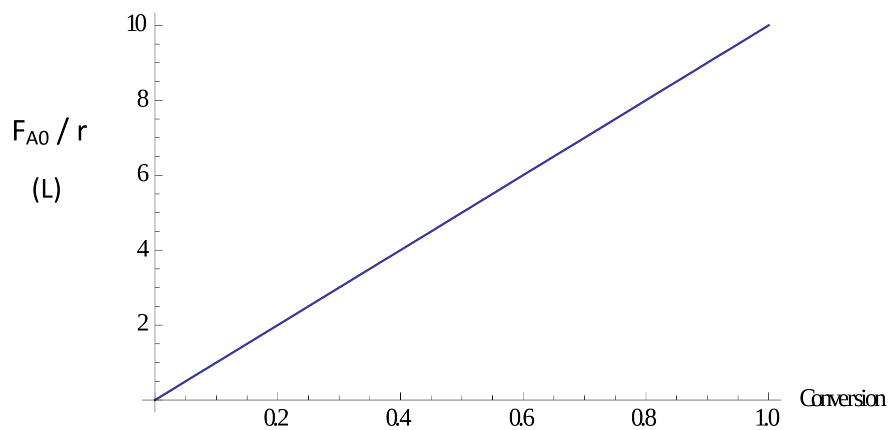
Please consider an enzymatic reaction with competitive inhibition. The reaction stoichiometry is

$$A + E \leftrightarrow I + P + E$$

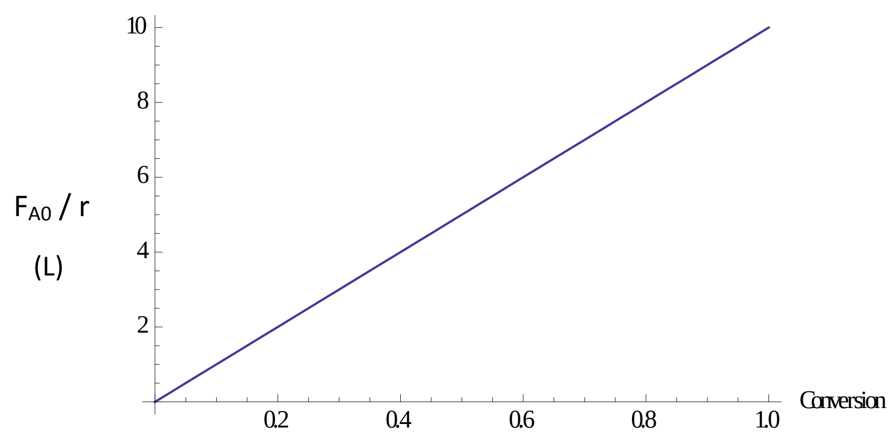
Where I is the inhibitor. The volumetric flow rate is 10 L min^{-1}. Levenspiel plots are provided for this problem below.

(a) Show and clearly label the volumes of a CSTR reactor and a PFR reactor required to reach a conversion of 0.8, using the templates below.

Show CSTR Work Here (part a)



Show PFR Work Here (part a)



(b) Which one single reactor would you use to minimize your reactor volume?

(c) What is the ratio of volumes of a CSTR and a PFR required to reach the same arbitrary conversion? Provide a physical explanation as to why this ratio is not unity (1 sentence).

Problem 4

A stirred tank reactor initially contains contaminants at 3 M concentration. To clean the CSTR for the reaction, it is flushed with a pure solvent stream at t=0. Assume the tank volume is constant and all liquids are incompressible.

(a) What are the limiting concentration of contaminants in this CSTR cleaning at short times and long times?

(b) What is the concentration of contaminant in the CSTR at $t=\tau$ (residence time).

(c) Sketch the contaminant concentration as a function of $t' = t/\tau$ (t = time and τ = residence time). Clearly label the concentration at $t' = 0$ and its asymptotic value at very long times.

(d) On the same plot as part (c), sketch the concentration of contaminant exiting a PFR as a function of t'. You may assume the PFR has the same residence time and the same initial contaminant concentration. Again, clearly label the concentration at $t'=0$ and its value at very long times. Also label on the plot for the PFR where $t' =1$.

Problem 5

Please provide concise answers to these unrelated (to each other) questions.

(a) The liquid-phase reaction A → B + C with $-r_A = kC_A^2$ is to be carried out in steady-state in an isothermal reactor. Should one use a CSTR or a PFR in order to achieve the highest possible conversion of A for a fixed space time? Explain physically why in a single sentence. How would your answer change if it is a gas phase reaction?

(b) You are given two CSTRs of equal volume to carry out a liquid phase reaction (A→ B) with a rate equation $r = k_1 C_A^2/(1+k_2 C_A)$. Would you arrange them in parallel or in series to reach the highest exit conversion of A? Explain physically why in a single sentence.

(c) A liquid phase reaction (A → B) is taking place in an isothermal isobaric batch reactor. What would happen to the total concentration of the system, concentration of A and concentration of B (increases, decrease or remain constant)? Justify your answer in a single sentence.