CBE 142: Chemical Kinetics & Reaction Engineering

Midterm #1
October 13th 2015

This exam is worth 120 points and 30% of your course grade. You have 80 minutes to complete this exam, so please manage time wisely. Please read through the questions carefully before giving your response. Make sure to SHOW ALL YOUR WORK and BOX your final answers! Answers without a clear and legible thought process will receive no credit.

Name: ____

Student ID: ____

Section (Day/GSI) that you **attend**: ____________________________

You are allowed one 8.5''x11'' sheet of paper (front and back) and a calculator for this exam. Any additional paper you wish to be graded must have your NAME and STUDENT ID written on each page.

Problem	**Max Points**	**Points Earned**
1	25	
2	25	
3	35	
4	35	

TOTAL : ____________

USEFUL INFORMATION

Quadratic Formula

Given $ax^2 + bx + c = 0$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Useful integrals

$$\int \frac{dx}{A + Bx} = \frac{1}{B}\ln(A + Bx) + C$$

Problem # 1. Basic Concepts in Reactor Design [25 pts]

Consider the irreversible liquid-phase reaction A + B → C. The reaction rate can be described by the rate law

$r = k_1 C_A^{-2} C_B$ for $X_A < 0.5$

$r = k_2 C_B$ for $X_A \geq 0.5$

were X_A is the overall conversion of A, C_A and C_B are the concentrations of A and B respectively, and k_1 and k_2 are rate parameters.

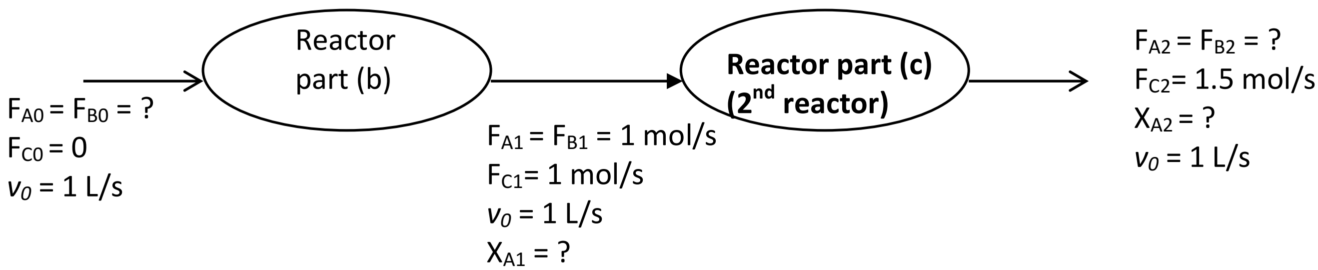
(a) What are the units of k_1 and k_2. [5 pts]

(b) We desire to obtain a conversion less than 0.5 in an isothermal, steady state reactor with equimolar feed of A and B (no C present in feed). For a given reactor volume, which type of reactor would give a higher conversion? [5 pt]

(A) An ideal PFR
(B) An ideal CSTR
(C) Both are equivalent

Explain physically why this is the case in a single sentence. Answers without explanation will receive no credit.

(c) The stream exiting the steady-state reactor in part (b) consists of 1 mol/s of A, 1 mol/s of B, and 1 mol/s of C. It is directly fed into a second steady-state isothermal reactor.

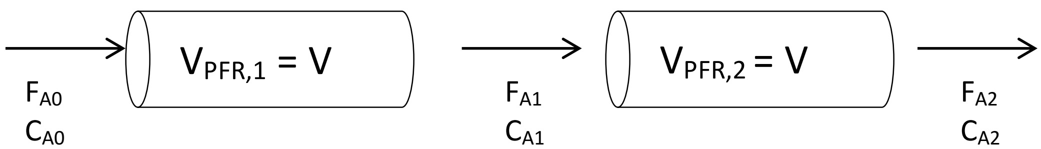


(i) Which one of the rate laws describes the kinetics for this second reactor? [5 pts]

(ii) The volumetric flow rate into the reactor is 1 L/s. The rate constant in the second reactor has a value of 1 (units are the relevant ones you found in part (a)). For the second reactor, what is the **volume** needed to achieve an exit stream of 1.5 mol/s of C in a **steady state CSTR vs.** a **steady state PFR**? If the volumes are different, please explain physically why they are different. [10 pts]

Problem #2. PFRs in series reactor design [25 pts]

Two *identical* steady-state, isothermal PFRs of unknown volumes $V_1 = V_2 = V$ are connected in series as shown in the following figure:



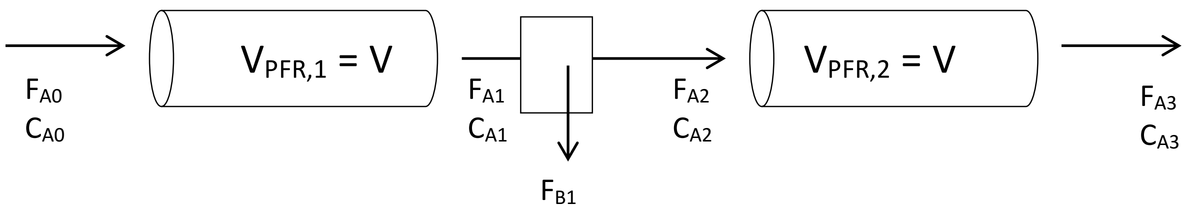
The following elementary, liquid-phase equilibrium reaction occurs:

$$A \overset{K}{\Leftrightarrow} B$$

where the equilibrium constant for this reaction, K, is equal to 5.8 and pure A is fed to the first reactor.

(a) The conversion of the first reactor, X_1, has been measured to be 0.55. What is the overall conversion of A, X_{ov}, at the outlet of the second reactor? [20 pts]

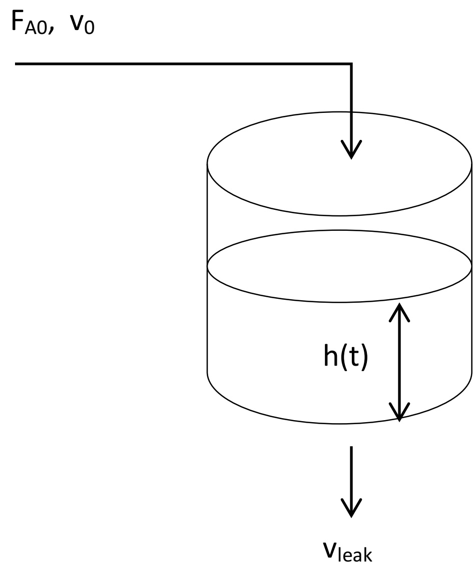
(b) Now, a very efficient separations unit is added in between the 2 PFR units such that *all* of the B is removed from the feed entering the second reactor.



What do you expect to happen to X_{ov} in this case, compared to the case you evaluated in part (a)? Explain in one sentence why this is so. Answers without a valid explanation will not receive credit. [5 pts]

Problem #3. Semi-batch reactor operation [35 pts]

The liquid phase, elementary, bimolecular rearrangement reaction 2A -> B + C with rate constant k_1 occurs in a cylindrical semi-batch reactor with cross-sectional area A_C. The initial liquid height is at h_0. F_{A0} mol/s of A flows into the reactor with a constant volumetric flow rate v_o. Unfortunately, the circular bottom of the vessel is leaky causing the contents to drain at a certain volumetric flow rate, v_{leak}:



The volumetric flow rate of the leak is proportional to the height of liquid in the tank:

$$v_{leak} = \alpha h$$

where α is a positive proportionality constant with proper units.

Note: All species are the same molecular weight and have the same liquid phase density

(a) Find an expression for the height of the liquid level in the tank as a function of time. [15 pts]

(b) Derive an expression for the evolution of the concentration of species A in time, $\frac{dC_A}{dt}$, in terms of C_A, h and its derivatives, and other constants. Do not worry about integrating it. [5 pts]

(c) After a very long time, what concentration of A do you expect to have in the tank? Show all work and explain all assumptions to receive credit. [15 pts]

Problem #4. PSSH and Reaction Mechanisms [35 pts]

The gas-phase reaction of chlorine with chloroform is described by the equation:

$$Cl_2 + CHCl_3 \rightarrow HCl + CCl_4$$

A proposed mechanism involves the following elementary steps:

$$Cl_2 \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} 2\,Cl\bullet \qquad \text{(step 1)}$$

$$Cl\bullet + CHCl_3 \xrightarrow{k_2} HCl + CCl_3\bullet \qquad \text{(step 2)}$$

$$CCl_3\bullet + Cl\bullet \xrightarrow{k_3} CCl_4 \qquad \text{(step 3)}$$

Species $Cl\bullet$ and $CCl_3\bullet$ are reactive intermediates.

(a) Assume that the first reaction step shown is quasi-equilibrated. Determine the rate law, r_{CCl4}, in terms of the rate constants and the concentrations of reactants and products. [15 pts]

(b) Now relax the assumption of quasi-equilibration on step 1. Using only the pseudo steady-state hypothesis for all reactive intermediates, determine the rate law, r_{CCl4}, in terms of the rate constants and the concentrations of reactants and products. [15 pts]

(c) What must be true in order for the expression from (b) to collapse to the expression in (a)? This answer provides the rigorous justification for QE on step 1. Draw a rate arrow diagram and provide a specific inequality. [5 pts]