CBE 142: Chemical Kinetics & Reaction Engineering

Midterm #1
October 9th 2014

This exam is worth 100 points and 20% of your course grade. Please read through the questions carefully before giving your response. Make sure to SHOW ALL YOUR WORK and BOX your final answers!

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	15	
3	25	
4	10	
5	25	

TOTAL : ______________

Problem #1 (25 points)

For parts (a) – (d): Write the correct choice and take one sentence to explain your answer. Be CONCISE. Only correct choices with clear and correct supporting explanation will be counted.

For part (e): Solve for a numerical value.

a) (4 pt) An isothermal, liquid-phase reaction of $2A \leftrightarrows 3C$ obeys the following rate equation: $-r_A = kC_A^{-0.5}$. For a given reactor volume V, and volumetric flow rate v_o, in which reactor will we obtain a higher conversion?
   A. Ideal PFR
   B. Ideal CSTR
   C. Both reactors are equivalent

   Choice (A, B, C): __________
   Explanation:

b) (4 pt) An isothermal, elementary gas-phase reaction, $P + Q \rightarrow 2R + S$ occurs in a BSTR. Which type of reactor will give us a higher conversion at a given clock time, t*?
   A. Constant volume ideal BSTR
   B. Constant pressure ideal BSTR
   C. Both reactors are equivalent

   Choice (A, B, C): __________
   Explanation:

c) (4 pt) Consider an isothermal, elementary gas-phase reaction, $P + Q \rightarrow 2R + S$ occurring in an isobaric reactor. Which type of reactor will give us a higher conversion at a given residence time, t*?
   A. Constant pressure ideal BSTR
   B. Constant pressure ideal PFR
   C. Both reactors are equivalent

   Choice (A, B, C): __________
   Explanation:

d) (4 pt) An isothermal, elementary, reversible gas-phase reaction, P + Q ⇄ 2R + S occurs in a BSTR. In which type of BSTR reactor will we have a higher equilibrium conversion?
   A. Constant volume BSTR
   B. Constant pressure BSTR
   C. Both cases are equivalent.

   Choice (A, B, C): __________
   Explanation:

(e) (9 pt) Consider the elementary, reversible gas phase reaction represented by:

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} 2\,C$$

The reaction is carried out in an isothermal, isobaric flow reactor. Pure A enters at 400 K and at 10 atm. The equilibrium constant (K_{eq}) is 1.25 mol*L^{-1}. Use R=0.082 L*atm*K^{-1}*atm^{-1} for the universal gas constant.

What is the equilibrium conversion?

Problem #2 (15 points)

Consider a gas-phase reaction occurring in a PFR:

$$A_{gas} + 2B_{gas} \longrightarrow 4D_{gas \to liq}$$

Species D is the only one that may condense. The following information is available:

- The inlet volumetric flow rate is ν_0= 5 L/min
- The inlet stream is equimolar in species A and B, F_{A0}=F_{B0}
- Your reactor is operating isobarically,, P_{total} = 4atm
- Your reactor is operating isothermally, T=300K
- The vapor pressure of species D at 300K, $P_{Vap,D}$ = 1atm

Base your conversion on the limiting reactant in the system.

a) (1 pt) What is the limiting reactant?

b) (4 pt) Create a stoichiometric table for all species A, B and D. Keep in mind the regimes without condensation and after D condenses.

c) (5 pt) At what conversion will condensation of species D begin? Show all work. Answers without clear reasoning receive zero credit.

d) (5 pt) After condensation, derive an expression for how the volumetric flow rate **ν** relates to conversion. Show all work. Answers without clear reasoning receive zero credit.

Problem #3 (25 points)

Consider the reaction:

$$A \rightarrow 2B + 2C, \; r_{net}$$

It consists of the following three elementary reactions:

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} I_1 + 2B$$

$$I_1 \overset{k_2}{\rightarrow} 2I_2$$

$$I_2 \overset{k_3}{\rightarrow} C$$

a) (3 pt) What are the σ values for each step? Draw a rate-arrow diagram involving r_1, r_{-1}, r_2, and r_3 and clearly show how these relate to r_{net}?

b) (5 pt) PSSH applies for all intermediate species, derive a rate expression for r_{net}.

c) (5 pt) In the case that QE applies for step one, derive the rate expression for r_{net}.

d) (7 pt) Compare your answer in parts b) and c), and use this to provide the rigorous justification for QE in this system.

e) (5 pt) Draw the rate-arrow diagram for the reaction sequence assuming that QE applies to step one. Clearly label all of the rates being graphed including their relationship to r_{net}.

f) (5 pt) Draw the rate-arrow diagram for the reaction sequence assuming now that step one is practically irreversible. Clearly label all of the rates being graphed including their relationship to r_{net}.

Problem #4 (10 points)

A differential volume element in an ideal PFR moves down the volume of the reactor according to a volumetric flow rate given by

$$v = \alpha V + \beta \qquad (\mathrm{m^3/s})$$

where α, β are constants and the flow rate is a function of V, the swept reactor volume (m^3).

For the following cases, express the total residence time of this volume element if the total PFR volume is V_f (m^3), in terms of the constants α, β, and V_f (m^3).

a) (1 pt) Case $\alpha = 0$

b) (9 pt) Case $\alpha > 0$

Problem #5 (25 points)

Consider the irreversible, liquid-phase reaction represented by:

$$2A + S \rightarrow B + S \qquad r_B = kC_AC_S$$

The reaction is carried out isothermally in a semibatch reactor. The reactor initially contains an initial volume V_0 of pure A at a concentration of C_{A0}. At t=0, a solution of S at C_{S0} is fed into the reactor with a constant volumetric flow rate of v_S. The reaction rate for species B is given above and is first order in A, first order in S with a rate constant of k. The density of the liquid for all species in the reactor can be assumed constant.

For parts (a)-(d), <u>your answers must be in terms of the given constants (C_{A0}, C_{S0}, k, V_0, v_S)</u>.

Hint: note that S is not produced or consumed in the reaction, but is present in the rate law.

a) (1 pt) What is r_A in terms of r_B?

b) (4 pt) Perform an overall mass balance to solve for volume (V) as a function of time.

c) (5 pt) Start with a mole balance for species S and solve for C_S as a function of time.

d) (15 pt) Start with a mole balance for species A and solve for C_A as a function of time. Remember to put your final answer in terms of the values listed above.

The following integrals may (or may not) come in handy. Note that they have already been evaluated for the bounds of x from [0, x].

$$\int_0^x \frac{x}{x^2+a^2}dx = \frac{1}{2}ln\left[\frac{|x^2+a^2|}{|a^2|}\right]$$

$$\int_0^x \frac{ax+b}{cx+d}dx = \frac{ax}{c} + \frac{ad-bc}{c^2}\ln\left[\frac{|d|}{|cx+d|}\right]$$

$$\int_0^x \frac{x}{ax+b}dx = \frac{x}{a} + \frac{b}{a^2}\ln\left[\frac{|b|}{|ax+b|}\right]$$

$$\int_0^x \frac{1}{(ax+b)(cx+d)}dx = \frac{1}{ad-bc}ln\left[\frac{|d(ax+b)|}{|b(cx+d)|}\right]$$

$$\int_0^x \frac{x}{(ax+b)(cx+d)}dx = \frac{1}{ad-bc}\left(\frac{b}{a}ln\left[\frac{|b|}{|ax+b|}\right] + \frac{d}{c}ln\left[\frac{|cx+d|}{|d|}\right]\right)$$