

ChE 344
Winter 2011
Mid Term Exam I

Thursday, February 17, 2011

Closed Book, Web, and Notes

Name_____

Honor Code_____

(sign at the end of exam)

1) ____/ 5 pts

2) ____/ 5 pts

3) ____/ 5 pts

4)____/ 15 pts

5) ____/ 5 pts

6) ____/ 5 pts

7)____/ 20 pts

8)____/ 20 pts

9)____/ 20 pts

Total ____/100 pts

_____ I have a Laptop with Polymath on it that I can bring to the 2nd Midterm Exam.

_____ I will need to use the computer lab for the 2nd Midterm Exam.

ChE 344

Exam I

1. Simpson's Three-eighths rule (4 points)

$$\int_{x_0}^{x_3} f(x) dx = \frac{3}{8} h [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

2. $y = (1 - \alpha W)^{1/2}$

$$\frac{dy}{dW} = -\frac{\alpha(1 + \epsilon X)}{2y} \left(\frac{T}{T_0} \right) \quad \text{where } \alpha = \frac{2\beta_0}{A_C \rho_C (1 - \phi) P_0}, \text{ and } \beta_0 = \frac{G(1 - \phi)}{g_C \rho_0 D_p \phi^3} \left[\frac{150(1 - \phi)\mu}{D_p} + 1.75G \right]$$

$$\frac{dy}{dW} = -\frac{\alpha}{2y} \left(\frac{F_T}{F_{T0}} \right) \left(\frac{T}{T_0} \right)$$

3. Integrals

$$\int_0^X \frac{dX}{1 - X} = \ln \frac{1}{1 - X}$$

$$\int_0^X \frac{1 + \epsilon X}{(1 - X)^2} dX = \frac{(1 + \epsilon)X}{1 - X} - \epsilon \ln \frac{1}{1 - X}$$

$$\int_0^X \frac{dX}{(1 - X)^2} = \frac{X}{1 - X}$$

$$\int_0^X \frac{(1 + \epsilon X)^2}{(1 - X)^2} dX = 2\epsilon(1 + \epsilon) \ln(1 - X) + \epsilon^2 X + \frac{(1 + \epsilon)^2 X}{1 - X}$$

$$\int_0^X \frac{dX}{1 + \epsilon X} = \frac{1}{\epsilon} \ln(1 + \epsilon X)$$

$$\int_0^W (1 - \alpha W)^{1/2} dW = \frac{2}{3\alpha} [1 - (1 - \alpha W)^{3/2}]$$

$$\int_0^X \frac{1 + \epsilon X}{1 - X} dX = (1 + \epsilon) \ln \frac{1}{1 - X} - \epsilon X$$

$$\int_0^X \frac{dx}{(1 - X)(\theta_B - X)} = \frac{1}{\theta_B - 1} \ln \frac{\theta_B - X}{\theta_B(1 - X)} \quad \theta_B \neq 1$$

$$\int_0^X \frac{dX}{aX^2 + bX + c} = \frac{-2}{2aX + b} + \frac{2}{b}$$

for $b^2 = 4ac$ where p and q are the roots of the equation.

$$aX^2 + bX + c = 0 \quad \text{i.e., } p, q = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\int_0^X \frac{dX}{aX^2 + bX + c} = \frac{1}{a(p - q)} \ln \left(\frac{q}{p} \frac{X - p}{X - q} \right) \quad \text{for } b^2 > 4ac \quad \int_0^X \frac{a + bX}{c + gX} dX = \frac{bX}{g} + \frac{ag - bc}{g^2} \ln \left[\frac{(c + gX)}{c} \right]$$

4. Finite Difference

First Point: $-\left. \frac{dC_A}{dt} \right|_{t_0} = - \left[\frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t} \right]$

Middle Points: $-\left. \frac{dC_A}{dt} \right|_{t_i} = - \left[\frac{C_{A(i+1)} - C_{A(i-1)}}{2\Delta t} \right]$

e.g., $-\left. \frac{dC_A}{dt} \right|_{t_3} = - \left[\frac{C_{A4} - C_{A2}}{2\Delta t} \right] = \frac{C_{A2} - C_{A4}}{2\Delta t}$

Last Point: $-\left. \frac{dC_A}{dt} \right|_{t_5} = - \left[\frac{C_{A3} - 4C_{A4} + 3C_{A5}}{2\Delta t} \right]$

5. Ideal Gas Constant

$$R = \frac{8.309 \text{ kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}}$$

$$R = \frac{1.987 \text{ BTU}}{\text{lb mol} \cdot ^\circ\text{R}}$$

$$R = \frac{0.73 \text{ ft}^3 \cdot \text{atm}}{\text{lb mol} \cdot ^\circ\text{R}}$$

$$R = \frac{8.3144 \text{ J}}{\text{mol} \cdot \text{K}}$$

$$R = 0.082 \frac{\text{liter} \cdot \text{atm}}{\text{mol} \cdot \text{K}} = \frac{0.082 \text{ m}^3 \cdot \text{atm}}{\text{kmol} \cdot \text{K}}$$

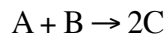
$$R = \frac{1.987 \text{ cal}}{\text{mol} \cdot \text{K}}$$

Volume of Ideal Gas

1 lb mol of an ideal gas at 32°F and 1 atm occupies 359 ft³.

(5 pts) 1) Mole Balances, Chapter 1

The reaction



takes place in an unsteady PFR. The feed is only A and B in equimolar proportions. Which of the following set of equations gives the correct mole balances on A, B and C. Species A and B are disappearing and Species C is being formed.

Circle the correct answer where all the mole balances are correct

(a)

$$F_{A0} - F_A - \int^V r_A dV = \frac{dN_A}{dt}$$

$$F_{B0} - F_B - \int^V r_A dV = \frac{dN_C}{dt}$$

$$-F_C + 2 \int^V r_A dV = \frac{dN_C}{dt}$$

(b)

$$F_{A0} - F_A + \int_0^V r_A dV = \frac{dN_A}{dt}$$

$$F_{B0} - F_B + \int^V r_A dV = \frac{dN_B}{dt}$$

$$F_C + \int^V r_C dV = \frac{dN_C}{dt}$$

(c)

$$F_{A0} - F_A + \int^V r_A dV = \frac{dN_A}{dt}$$

$$F_{B0} - F_B + \int^V r_A dV = \frac{dN_B}{dt}$$

$$-F_C - 2 \int^V r_A dV = \frac{dN_C}{dt}$$

$$F_{A0} - F_A - \int^V r_A dV = \frac{dN_A}{dt}$$

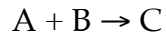
$$F_{B0} - F_B - \int^V r_A dV = \frac{dN_B}{dt}$$

$$-F_C + \int^V r_C dV = \frac{dN_C}{dt}$$

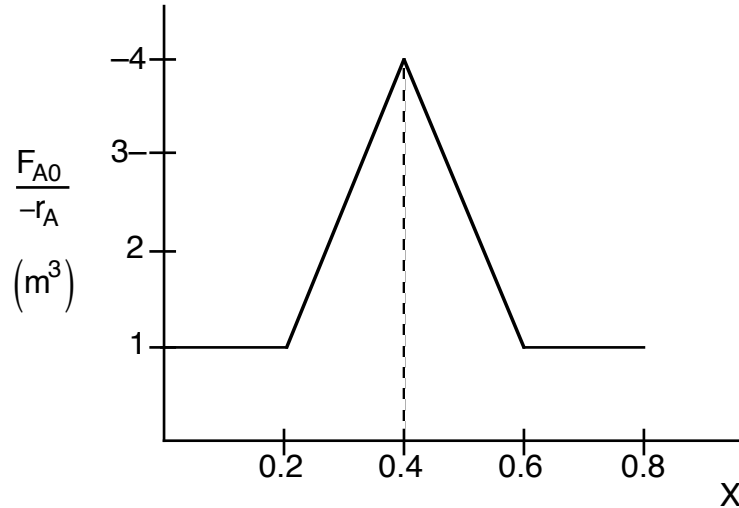
(d)

(5 pts) 2) Sizing, Chapter 2

For the gas phase reaction



equimolar amounts of A and B are to be fed, i.e., $y_{A0} = 0.5$ and $\delta \neq 0$. The following the Levenspiel plot was constructed for a temperature of $T = 318\text{K}$ and entering pressure of $P_0 = 10\text{ atm}$.



Note: $\delta \neq 0$

(a) What reactor type and size would you use to achieve 40% conversion?

Reactor Type _____ Volume _____

(b) What reactor type and size would you use to achieve 60% conversion?

Reactor Type _____ Volume _____

(c) What reactor type and size would you use to achieve 20% conversion?

Reactor Type _____ Volume _____

(d) What reactor type and size would you use to increase the conversion from 60% to 80%?

Reactor Type _____ Volume _____

Note: If more than one reactor type would work for any part (a – d), explain.

(5 pts) 3) **Rates, Chapter 3**

Determine the rate law for the reaction described in each of the cases below. The rate laws should be elementary as written for reactions that are of the form either $A \rightarrow B$ or $A + B \rightarrow C$

(a) The units of the specific reaction rate are

$$k = \left[\frac{\text{dm}^3}{\text{mol} \cdot \text{h}} \right]$$

Law _____

(b) The units of the specific reaction rate are

$$k = \left[\frac{\text{mol}}{\text{dm}^3 \cdot \text{h}} \right]$$

Law _____

(c) The units of the specific reaction rate are

$$k = \left[\frac{\text{mol}}{\text{kg cat} \cdot \text{h}(\text{atm})^2} \right]$$

Law _____

(d) The units of the specific reaction rate are

$$k = \left[\frac{1}{\text{h}} \right]$$

Law _____

(15 pts) 4) i>Clickers Chapters 4 and 5

(2 pts) 4a) Consider the gas-phase elementary reaction



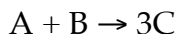
which takes place in a PFR in which R and inert I are fed. If the entering concentration of R is cut by a factor of 5 while maintaining a constant entering volumetric flow rate, v_0 , how will the conversion change?

Circle the correct answer.

- A) X won't change
- B) X will increase
- C) X will decrease

Explain_____

(3 pts) 4b) The liquid phase reaction



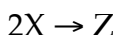
follows an elementary rate law and is carried out in a constant volume batch reactor with stoichiometric feed. For a batch reaction time of one hour the conversion is 50%. If the same reaction is carried out in a PFR at the same temperature in which there is no pressure drop, for the same space time of one hour would the conversion be

Circle the correct answer.

- A) $X > 50\%$
- B) $X < 50\%$
- C) $X = 50\%$
- D) Insufficient information to answer definitively

Explain_____

(2 pts) 4c) For the isothermal, elementary gas-phase reaction



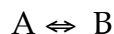
how does the PFR volume required for a given conversion change with increasing mole fraction, y_{X0} , of X when the inlet concentration of X and inlet total volumetric flow rate remain constant? There is no pressure drop and only X and Inert I enter the reactor.

Circle the correct answer.

- A) V increases
- B) V decreases
- C) No change in V
- D) Insufficient information to answer definitively

Explain_____

- (2 pts) 4d) If the following liquid-phase reaction is elementary and reversible, what is the rate expression in terms of conversion when equimolar amounts of A and B are fed to the reaction?

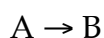


Circle the correct answer.

A) $-r_A = kC_{A0} \frac{[1-X]}{K_C X}$ C) $-r_A = kC_{A0} \left([1-X] - \frac{1+X}{K_C} \right)$
B) $-r_A = kC_{A0} [1-X]^2$ D) $-r_A = kC_{A0} \left(1-X \left[1 + \frac{1}{K_C} \right] \right)$

Explain _____

- (3 pts) 4e) Consider the reaction



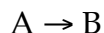
If the diameter of a PBR is doubled while keeping the turbulent flow mass flow rate, $\dot{m}$, constant, what can be said about that factor by which the rate of pressure drop (dy/dW) will be lowered?

Circle the correct answer.

- A) It will be lowered by a factor of 4
B) It will be lowered by a factor of 16
C) It will be lowered by a factor of 32
D) It will be lowered by a factor of 48 or more

Explain _____

- (3 pts) 4f) In a particular differential reactor experiment for the reaction



the entering volumetric flow rate is doubled, leaving all other variables the same. How would you expect the measured outlet flow rate of B, to change under conditions of differential reactor conversion?

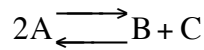
Circle the correct answer.

- A) Molar flow rate of product will go up
B) Molar flow rate of product will go down
C) No Change

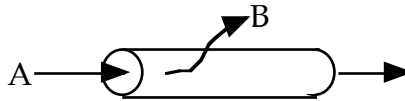
Explain _____

(5 pts) 5) Membrane Reactors, Chapter 6

(2 pts) 5a) Consider the gas phase reaction

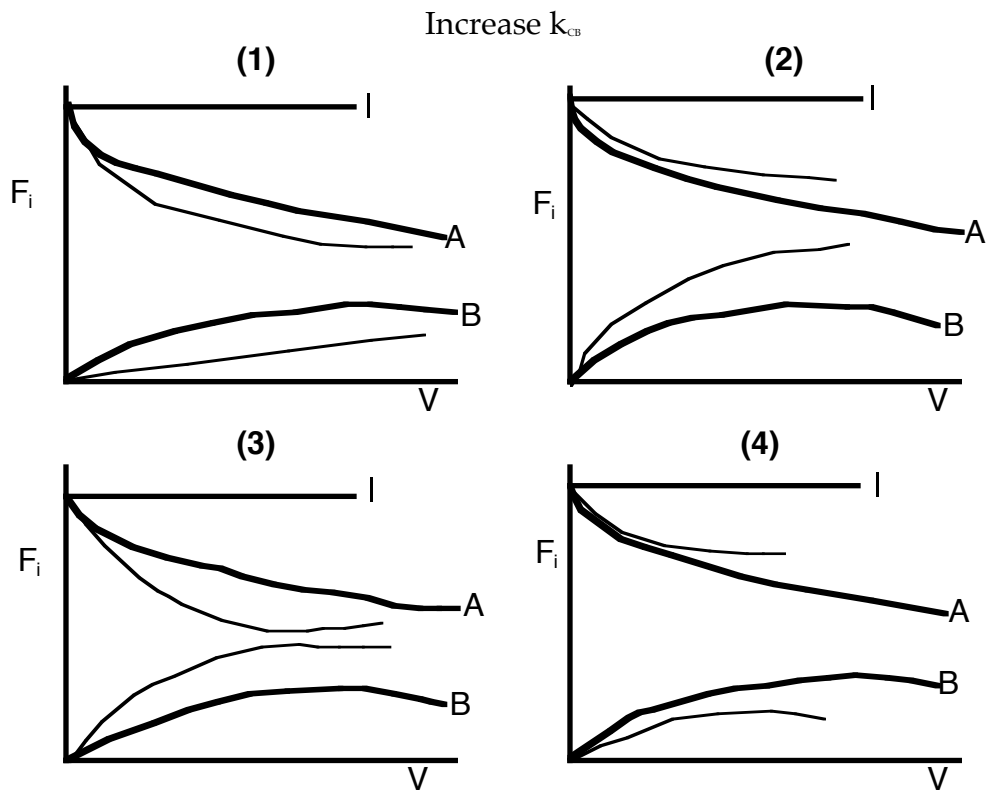


On the figure below is a sketch the molar flow rates F_A , F_B , and F_i for species A and B as a function of membrane volume. The dark lines, A and B, represent the base case while the lighter lines represents possible profiles when the mass transfer coefficient for B, k_{CB} , is increased. Which figure correctly corresponds to an increase in the mass transfer coefficient k_{CB} ?



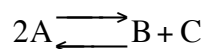
Circle the correct answer.

- A) 1
- B) 2
- C) 3
- D) 4

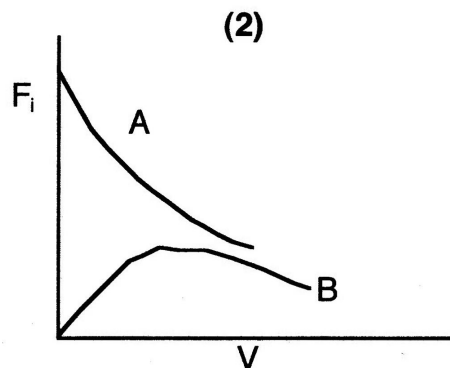
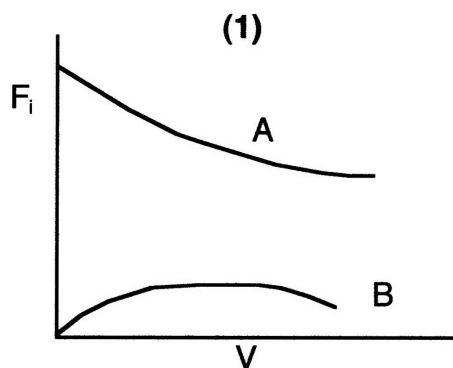
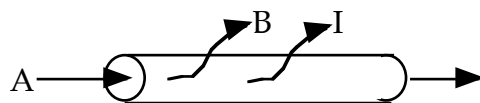


Explain _____

(3 pts) 5b) Membrane Reactor 50% A and 50% I inerts



Both B and inerts I diffuse out. Which of the following figures has the greatest mass transfer coefficient for the inerts, k_G for the rate of removal of inerts? All other constants remain the same.



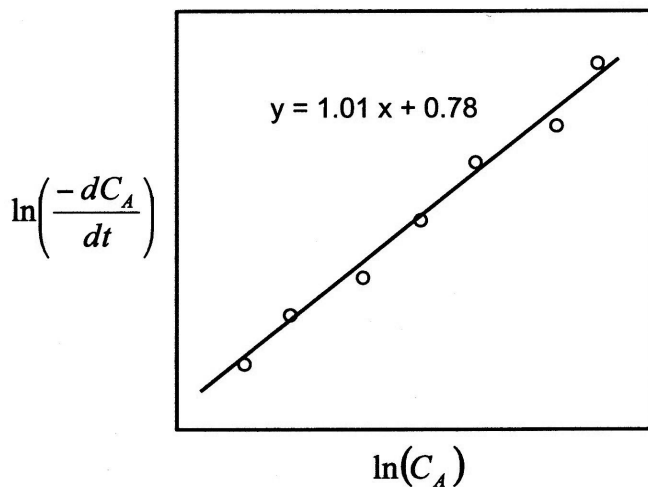
Circle the correct answer.

- A) 1
- B) 2

Explain _____

(5 pts) 6) Analysis of Data, Chapter 7

(2 pts) 6a) From the following plot, what is the reaction order with respect to A?

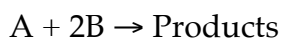


Circle the correct answer.

- A) 0
- B) 0.5
- C) 0.78
- D) 1
- E) 2

Explain _____

(3 pts) 6b) The following reaction, batch experiments are conducted to evaluate the reaction kinetics. The slope of a $\ln(r_v)$ versus $\ln(C_v)$ plot is measured to be 1.02 and the intercept is 0.42 when A is in great excess. What is the *overall* reaction order?



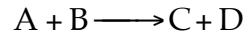
Circle the correct answer.

- A) 0.42
- B) 1.02
- C) 1.44
- D) Can't tell on the basis of this experiment

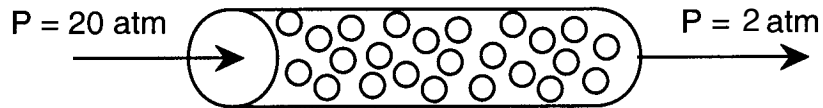
Explain _____

(20 pts) 7) Pressure Drop, Chapter 5

The gas phase reaction



is carried out isothermally at 227°C in a packed bed reactor with 100 kg of catalyst. The reaction is first order in A and first order in B.



The entering pressure was 20 atm and the exit pressure is 2 atm. The feed is equal molar in A and B and is in the flow in the turbulent regime with $F_{A0} = 10 \text{ mol/min}$ and $C_{A0} = 0.244 \text{ mol/dm}^3$. Currently 80% conversion is achieved. Intra particle diffusion effects in the catalyst particles can be neglected.

(a) What is the specific reaction rate?

$k = \underline{\hspace{2cm}}$

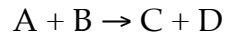
(b) What would be the conversion if the particle size were doubled and there are no internal mass transfer limitations?

$X = \underline{\hspace{2cm}}$

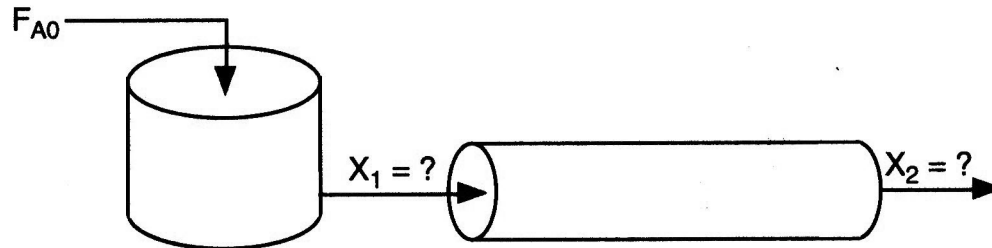
(20 pts) 8) *Modified California Problem P5-20_b*



The elementary gas phase reaction



takes place isobarically and isothermally in a PFR where 50% conversion is achieved. The feed is equimolar in A and B. It is proposed to put a CSTR of equal volume upstream, i.e.,



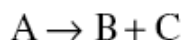
of the PFR. What will be the intermediate and exit conversions X_1 and X_2 respectively? The entering flow rates and all other variables remain the same as that for the single PFR.

$X_1 =$ _____

$X_2 =$ _____

(20 pts) 9) **P5-9. Study Problem on Syllabus.**

The gas phase reaction



follows an elementary rate law and is to be carried out first in a PFR and then in a separate experiment in a CSTR. When Pure A is fed to a 10 dm³ PFR at 300K and a volumetric flow rate of 5 dm³/s, the conversion is 80%. When a mixture of 50% A and 50% inert (I) is fed to a 10 dm³ CSTR at 320K and a volumetric flow rate of 5 dm³/s the conversion is also 80%. What is the activation energy in cal/mol?

E = _____ cal/mol

