

ChE 344
Winter 2013
Mid Term Exam I + Solution
Tuesday, February 26, 2013
Closed Book, Web, and Notes

Name _____

Honor Code _____

(Sign at the end of exam period)

- 1) ____ / 5 pts
- 2) ____ / 5 pts
- 3) ____ / 5 pts
- 4) ____ / 5 pts
- 5) ____ / 5 pts
- 6) ____ / 5 pts
- 7) ____ / 10 pts
- 8) ____ / 15 pts
- 9) ____ / 20 pts
- 10) ____ / 25 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

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

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

$$\int_{x_1}^{x_2} \frac{dx}{(1 - x)^2} = \frac{1}{1 - x_2} - \frac{1}{1 - x_1}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

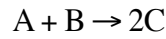
Volume of Ideal Gas

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

1 g mol of an ideal gas at 0°C and 1 atm occupies 22.4 dm³.

(5 pts) 1) **Chapter 1 Mole Balances**

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)

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

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

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

Ans: Wrong sign for r_A , should be $+\int^V r_A dV$

(b)

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

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

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

Ans: Wrong sign for F_C , should be $-F_C$

(c)

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

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

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

Ans: All are correct.

(d)

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

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

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

Ans: Wrong sign for $-r_A$, should be $+\int^V r_A dV$

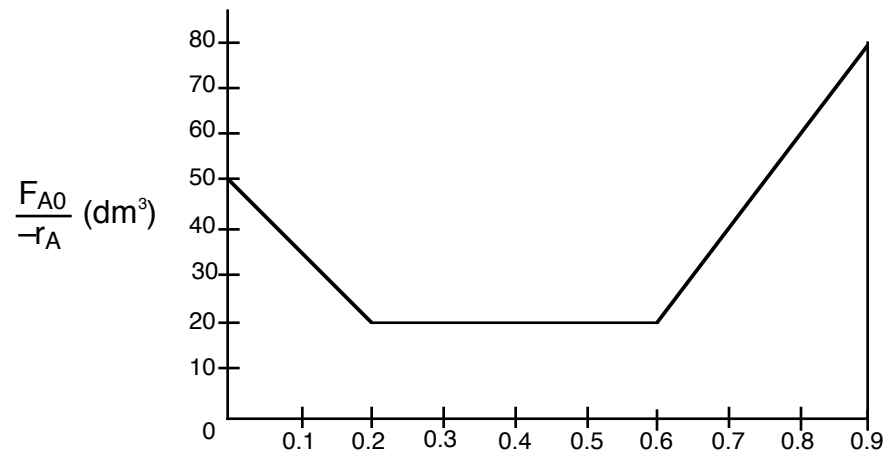
Solution

Answer is (c).

(5 pts) 2) The reaction



takes place in the gas phase

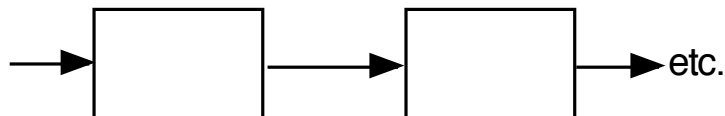


You have up to \$10,000 to use to purchase a reactor from those given below.

Reactor Type	Number	Volume (dm^3)	Cost
CSTR	1	2	\$1,000
CSTR	1	4	\$2,000
PFR	1	4	\$2,000
CSTR	1	6	\$4,000
CSTR	1	12	\$8,000
PFR	1	12	\$6,000

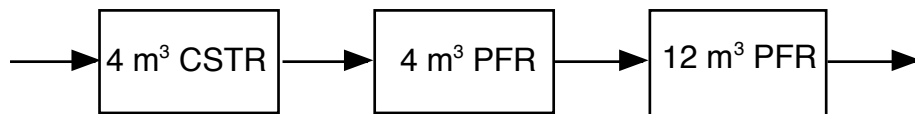
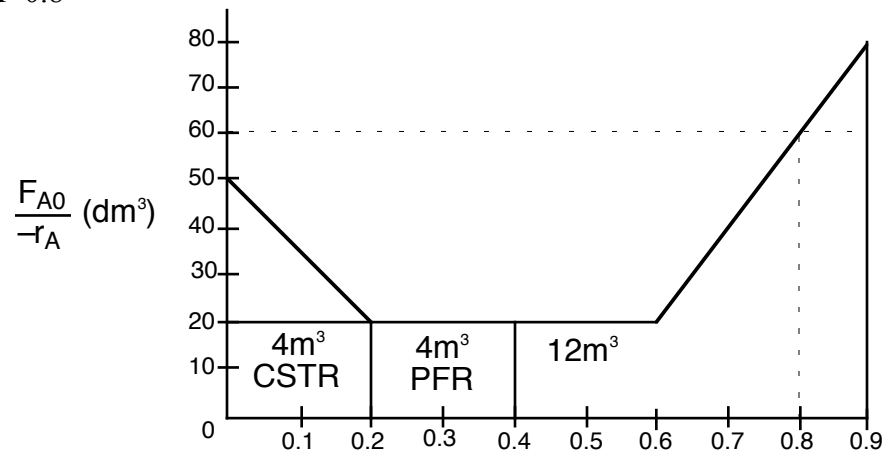
What reactors do you choose, how do you arrange them and what is the highest conversion you can get for \$10,000? Approximately what is the corresponding highest conversion $X = \underline{\hspace{2cm}}$ with your arrangement of reactors?

Scheme and Volume



Solution

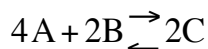
$X=0.8$



(5 pts) 3) **Chapter 3 Rate Laws**

Write the rate law in terms of concentrations for each of the following

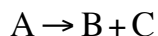
(a) The reaction



follows an elementary rate law. The feed is equal molar in A and B

$$-r_A = \underline{\hspace{2cm}}$$

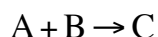
(b) The reaction



is pseudo first order at high concentrations of A and pseudo second order at low concentrations of A

$$-r_A = \underline{\hspace{2cm}}$$

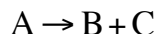
(c) The reaction



is first order in A and overall zero order.

$$-r_A = \underline{\hspace{2cm}}$$

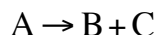
(d) The reaction



is carried out in a constant volume batch reactor and where the reciprocal of the concentration of A varies linearly with time.

$$-r_A = \underline{\hspace{2cm}}$$

(e) The reaction



is carried out in a constant volume batch reactor and where the concentration of A decreases linearly with time.

$$-r_A = \underline{\hspace{2cm}}$$

Solution

$$(a) \quad -r_A = k_A \left[C_A^4 C_B^2 - \frac{C_C^2}{K_C} \right]$$

$$(b) \quad -r_A = \frac{k_1 C_A^2}{1 + k_2 C_A}$$

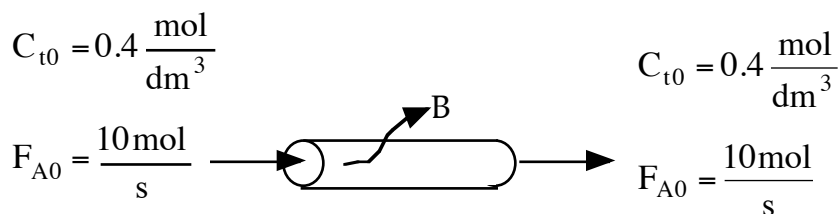
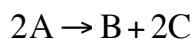
$$(c) \quad -r_A = \frac{k_1 C_A}{C_B}$$

$$(d) \quad -r_A = k C_A^2$$

$$(e) \quad -r_A = k$$

(5 pts) 4) **What four things are wrong with this solution?**

The gas phase elementary reaction



is carried out in a membrane reactor in which there is pressure drop with $\alpha = 0.019 \text{ kg}^{-1}$. An equal molar feed of A and inerts, I, enter the reactor and only species B can exit the membrane. Plot the conversion of A down the the membrane reactor containing 50 kg of catalyst. The specific reaction rate is $k_A = 2.5 \text{ dm}^6/\text{mol}/\text{kg}/\text{s}$, and the mass transfer coefficient $k_C = 1.5 \text{ dm}^3/\text{kg} \cdot \text{s}$,

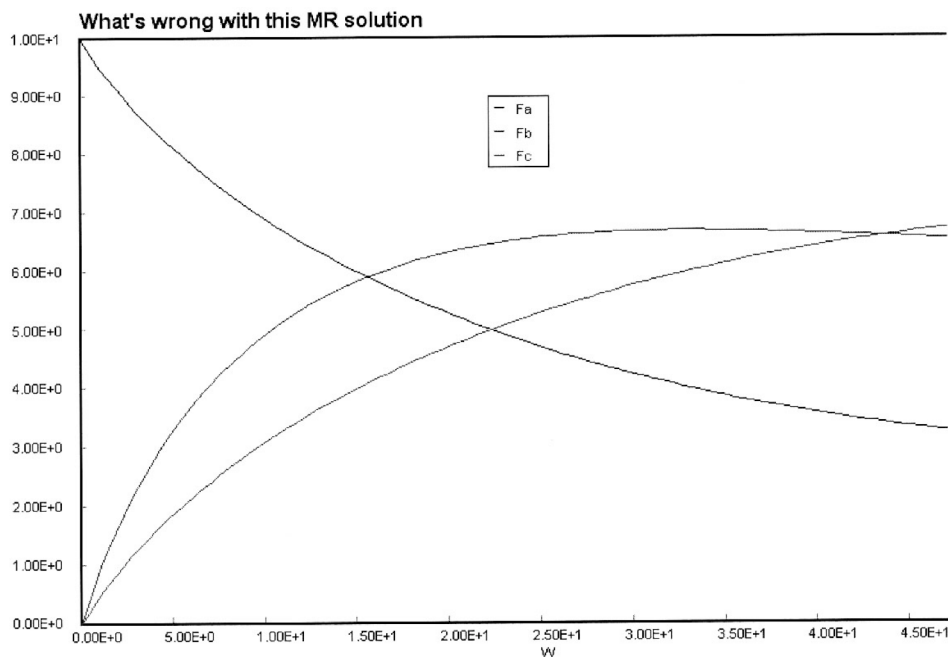
Solution

Differential equations

- 1 $d(F_A)/d(W) = r_A$
- 2 $d(F_B)/d(W) = r_B - R_B$
- 3 $d(F_C)/d(W) = r_C$

Explicit equations

- 1 $F_t = F_A + F_B + F_C$
- 2 $k_A = 2.5$
- 3 $C_{t0} = 0.4$
- 4 $\alpha = 0.019$
- 5 $y = (1 - \alpha \cdot W)^{0.5}$
- 6 $C_B = C_{t0} \cdot F_B \cdot y / F_t$
- 7 $C_A = C_{t0} \cdot F_A \cdot y / F_t$
- 8 $r_B = k_A \cdot C_A$
- 9 $r_A = -r_B/2$
- 10 $r_C = -r_A$
- 11 $k_C = 1.5$
- 12 $R_B = k_C \cdot C_B$



Identify 4 things that are incorrect or may not be included with this solution?

Reads

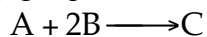
Should Read

- | | | |
|-----------|-------|-------|
| 1. Line # | _____ | _____ |
| 2. Line # | _____ | _____ |
| 3. Line # | _____ | _____ |
| 4. Line # | _____ | _____ |

Actual Solution

- | | | | |
|----|----------------------------|-----------|---|
| 1) | $r_B = -kC_A$ | should be | $r_A = -kC_A^2$ |
| 2) | $r_A = -\frac{r_B}{2}$ | should be | $r_B = -\frac{r_A}{2}$ |
| 3) | $F_T = F_A + F_B + F_C$ | should be | $F_T = F_A + F_B + F_C + F_I$ |
| 4) | $y = (1 - \alpha w)^{1/2}$ | should be | $\frac{dy}{dW} = -\frac{\alpha}{2y} \frac{F_T}{F_{T0}}$ |

(5 pts) 5) **Problem Statement.** The elementary gas phase reaction



is carried out in a packed bed reactor. Calculate the exit conversion from a PBR packed with 800 kg of catalyst. The feed is stoichiometric.

Additional Information

$$\alpha = 0.001 \text{ kg}^{-1}$$

$$C_{A0} = 0.04 \text{ mol/dm}^3$$

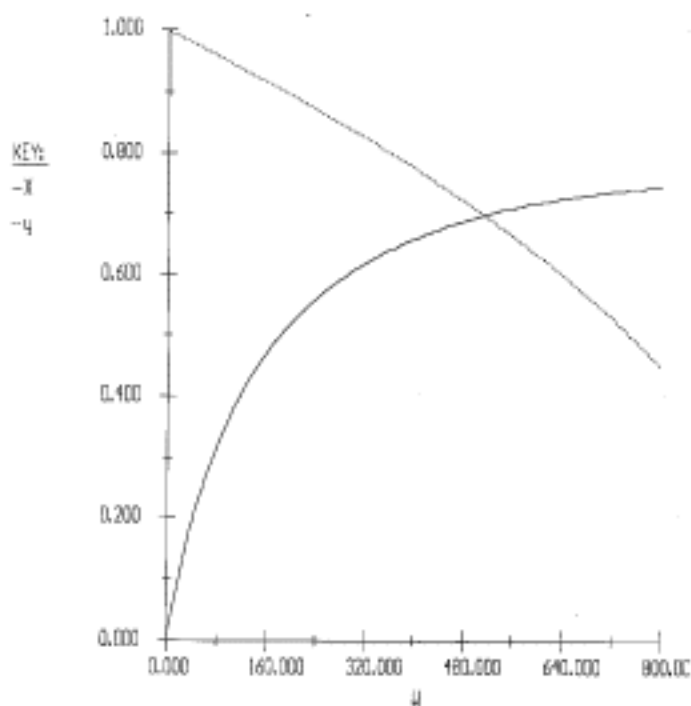
$$k = 3.0 \text{ dm}^6/\text{mol}^2 \cdot \text{s}$$

$$v_0 = 20 \text{ dm}^3/\text{s}$$

Solution

Equations:

- 1 $d(X)/d(W) = -r_{\text{prime}}/F_{A0}$
- 2 $k=3$
- 3 $C_{A0}=0.04$
- 4 $\alpha=0.001$
- 5 $v_0=20$
- 6 $y=(1-\alpha \cdot W)^{0.5}$
- 7 $F_{A0}=C_{A0} \cdot v_0$
- 8 $C_A=C_{A0} \cdot (1-X) \cdot y$
- 9 $C_B=C_{A0} \cdot (1-X) \cdot y$
- 10 $r_{\text{prime}}=-k \cdot C_A \cdot C_B$
- 11 $W_0 = 0, \quad W_f = 800$



What four things are wrong or may not be included with this solution?

	Reads	Should Read
1. Line #	_____	_____
2. Line #	_____	_____
3. Line #	_____	_____
4. Line #	_____	_____

Solution

1) The rate law is incorrect. It should be:

$$r_A = -kC_A C_B^2$$

2) The concentrations are incorrect, the feed is stoichiometric.

$$\theta_B = 2$$

3) The volume change was not included.

$$v = v_o(1 + \epsilon X) \frac{P_0}{P} \frac{T}{T_0} = v_o(1 + \epsilon X)$$

$$\epsilon = y_{A0}\delta = \frac{1}{3}(1 - 1 - 2) = -\frac{2}{3}$$

$$C_A = C_{A0} \frac{\left[\frac{(1-X)}{\left(1 - \frac{2}{3}X\right)} \right]}{\left(1 - \frac{2}{3}X\right)} = \frac{2C_{A0}(1-X)}{\left(1 - \frac{2}{3}X\right)} y$$

4) The equation for y is incorrect. There is volume change and $y = (1 - \alpha W)^{1/2}$ can only be used when $\epsilon = 0$. Therefore, the form of the momentum balance that must be used is

$$\frac{dy}{dw} = -\frac{\alpha(1 + \epsilon X)}{2y}$$

Corrected Solution

Equations:

$$d(y)/d(W) = -\alpha/2/y * (1 + \epsilon X)$$

$$d(X)/d(W) = -r_{\text{prime}}/F_{A0}$$

$$\alpha = 0.001$$

$$\epsilon = -2/3$$

$$k = 3$$

$$C_{A0} = 0.04$$

$$v_o = 20$$

$$F_{A0} = C_{A0} * v_o$$

$$C_A = C_{A0} * (1 - X) * y / (1 + \epsilon X)$$

$$C_B = C_{A0} * 2 * (1 - X) * y / (1 + \epsilon X)$$

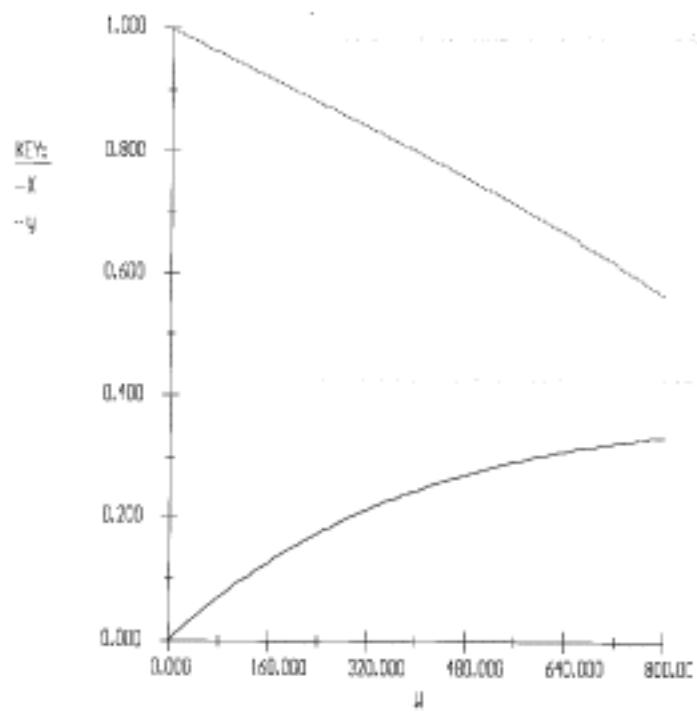
$$r_{\text{prime}} = -k * C_A * C_B^2$$

$$W_0 = 0, \quad W_f = 800$$

Initial value

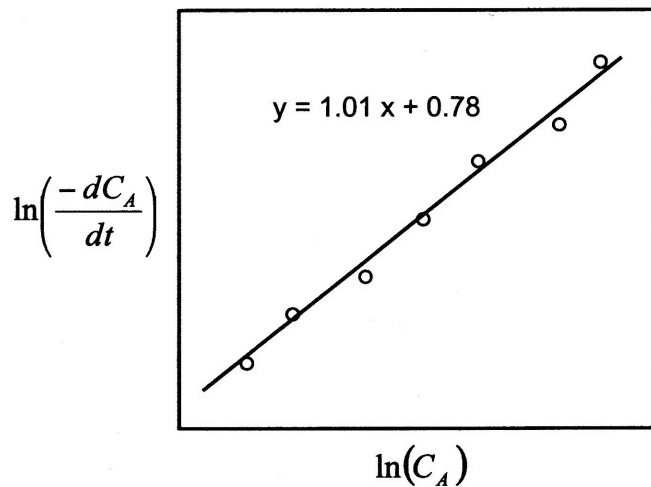
1

0



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

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



Circle the correct answer.

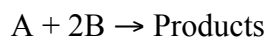
- A) 0
- B) 0.5
- C) 0.78
- D) 1
- E) 2

Explain _____

Solution

D) 1
Slope = 1.01 $\approx$ 1

(3 pts) 6b) The following reaction, batch experiments are conducted to evaluate the reaction kinetics. The slope of a $\ln(r_B)$ versus $\ln(C_B)$ 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 _____

Solution

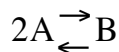
D) Can't tell on the basis of this experiment

$$-r_A = \frac{-r_B}{2} = kC_A^\alpha C_B^\beta = \ln\left(\frac{-r_B}{2}\right) = \ln k + \alpha \ln C_A + \beta \ln C_B$$

Both C_A and C_B vary, need to find α by varying C_A

(10 pts) 7) **Chapter 4 Stoichiometry**

The reversible reaction



is carried out in a flow reactor where pure A is fed at a concentration of 4.0 mol/dm^3 . If the equilibrium conversion is found to be 60%

(a) What is the equilibrium constant, K_C if the reaction is a gas phase reaction?

Gas $K_C =$ _____

(b) What is the K_C if the reaction is a liquid phase reaction?

Liquid $K_C =$ _____

Solution

(a) Gas

$$-r_A = k \left[C_A^2 - \frac{C_B}{K_C} \right]$$

At equilibrium, $-r_A = 0$

$$K_{Ce} = \frac{C_{Be}}{C_{Ae}^2}$$

$$\delta = \frac{1}{2} - 1 = -\frac{1}{2}, y_{A0} = 1, \varepsilon = -\frac{1}{2}$$

$$C_A = C_{A0} \left[\frac{(1-X)}{(1+\varepsilon X)} \right]$$

$$C_B = C_{A0} \left[\frac{\frac{1}{2}X}{(1+\varepsilon X)} \right]$$

$$\begin{aligned} K_{Ce} &= \frac{C_{A0} \left[\frac{\frac{1}{2}X_e}{(1+\varepsilon X_e)} \right]}{C_{A0}^2 \left[\frac{(1-X_e)}{(1+\varepsilon X_e)} \right]^2} = \frac{X_e(1+\varepsilon X_e)}{2C_{A0}(1-X_e)^2} \\ &= \frac{X_e(1-0.5X_e)}{2C_{A0}(1-X_e)^2} = \frac{0.6(0.7)}{8(0.4)^2} \\ &= 0.328 \text{ dm}^3 / \text{mol} \end{aligned}$$

(b) Liquid

$$-r_A = k \left[C_A^2 - \frac{C_B}{K_C} \right]$$

At equilibrium, $-r_A = 0$

$$K_{Ce} = \frac{C_{Be}}{C_{Ae}^2}$$

$$C_A = C_{A0}(1 - X)$$

$$C_B = C_{A0} \frac{1}{2} X$$

$$\begin{aligned} K_{Ce} &= \frac{C_{A0} \left[\frac{1}{2} X_e \right]}{C_{A0}^2 (1 - X_e)^2} = \frac{X_e}{2 C_{A0} (1 - X_e)^2} \\ &= \frac{0.6}{8(0.4)^2} \\ &= 0.469 \text{ dm}^3 / \text{mol} \end{aligned}$$

(15 pts) 8) **Multiple Choice (15 points)**

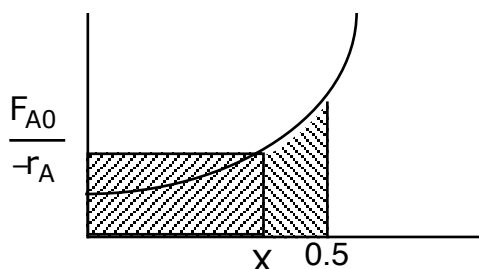
(3 pts) 8a) A reversible, liquid-phase reaction that is first order in both directions proceeds to 50% conversion in a PFR operating isothermally, isobarically, and at steady state. What conversion would be obtained in a CSTR with the same volume and feed stream and operating at exactly the same temperature and pressure?

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

Reason: _____

Solution

8a) Answer: (B) $X < 50\%$



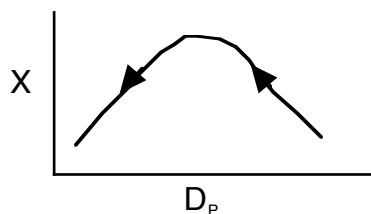
(3 pts) 8b) The gas reaction $A + B \rightarrow C$ is carried out in a packed bed where there is pressure drop. Currently 40% conversion is achieved. If the catalyst weight remains the same, but the particle size is increased, then the conversion would

- (A) increase (B) decrease (C) remain the same (D) insufficient information to answer definitively

Reason: _____

Solution

8b) Answer: (D) insufficient information to tell. You don't know which part of the curve you are on.

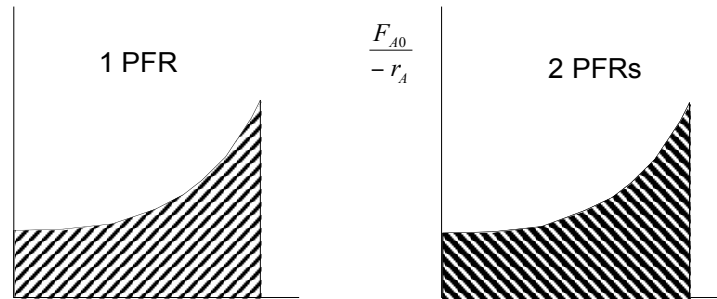


(3 pts) 8c) For an irreversible second order reaction 50% conversion is currently achieved in one PFR of $1,000 \text{ dm}^3$. It is proposed to use two 500 dm^3 PFRs placed in series. The exit conversion for the two PFRs will be

- (1) $> 50\%$ (2) 50% (3) $50\% <$ (4) Can't tell without the rate law

Solution

8c) Answer: (2) 50%



(3 pts) 8d) The rate constant for an irreversible, heterogeneously catalyzed, gas-phase, second order reaction, $A \rightarrow \text{Product(s)}$, was determined to be 0.234 from experimental data in a packed-bed reactor. The person analyzing the experimental failed to include the large pressure drop in the reactor in his analysis. If the pressure drop were properly accounted for, the rate constant would be

- (1) >0.234 (2) <0.234 (3) 0.234 (4) insufficient information to answer definitively
-
-
-

Solution

8d) Answer: (1) >0.234

$$-r_A = k C_{A0}^2 (1-X)^2 y^2$$

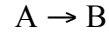
$$-r_A \propto k y^2$$

$$y^2 < 1$$

$$k^{true} y^2 = k = 0.234$$

$$k^{true} = \frac{0.234}{y^2} > 0.234$$

(3 pts) 8e) 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 _____

Solution

8e) Answer: D

It will be lowered by more than a factor of 48.

$$G \sim \frac{\dot{m}}{D^2}, \quad A_C \sim \pi D^2$$

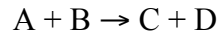
$$\alpha \sim \frac{G^2}{A_C} \sim \left(\frac{1}{D^4} \right) \left(\frac{1}{D^2} \right) = \frac{1}{D^6}$$

$$\alpha_2 = \alpha \left(\frac{D_1}{D_2} \right)^6 = \alpha_1 \left(\frac{1}{2} \right)^6 = \frac{\alpha_1}{64}$$

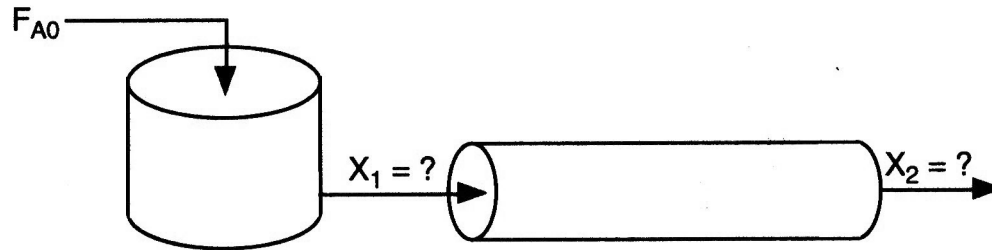
(20 pts) 9) **Study Problem P5-20_B, Modified California Problem**



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.

$$X_1 = \underline{\hspace{2cm}}$$

$$X_2 = \underline{\hspace{2cm}}$$

Solution

Case 1

$$\text{Mole Balance } \frac{dX}{dV} = -r_A$$

$$\text{Rate Law } -r_A = kC_A C_B$$

Stoichiometry

$$\text{Gas } \delta = 0, \Theta_B = 1$$

$$C_A = C_{A0}(1 - X)$$

$$C_B = C_{A0}(1 - X)$$

$$\text{Combine } -r_A = kC_{A0}^2(1 - X)^2$$

$$\frac{dX}{dV} = \frac{kC_{A0}^2(1 - X)^2}{F_{A0}}$$

$$\frac{dX}{(1 - X)^2} = \frac{kC_{A0}^2}{F_{A0}} dV$$

$$V = 0, \quad X = 0$$

$$V = V, \quad X = 0.5$$

$$\int_0^X \frac{dX}{(1-X)^2} = \frac{X}{1-X} = \frac{kC_{A0}^2}{F_{A0}} V$$

$$\frac{kC_{A0}^2}{F_{A0}} V = \frac{0.5}{1-0.5} = 1$$

Case 2

$$(1) V_{CSTR} = \frac{F_{A0}X}{-r_A}$$

(2) & (3) Rate Law, Stoichiometry same as Case 1

$$V_{CSTR} = \frac{F_{A0}X_1}{kC_{A0}^2(1-X_1)^2}$$

$$\frac{VkC_{A0}^2}{F_{A0}} = 1 = \frac{X_1}{1-2X_1+X_1^2}$$

$$1-2X_1+X_1^2 = X_1$$

$$X_1^2 - 3X_1 + 1 = 0$$

$$X_1 = \frac{3 \pm \sqrt{9-4}}{2} = \frac{3-\sqrt{5}}{2} = \frac{3-2.24}{2} = 0.38$$

$$\text{PFR } X_1 = 0.38$$

$$\frac{dX}{dV} = \frac{kC_{A0}^2(1-X)^2}{F_{A0}}, \quad \int_{X_1}^{X_2} \frac{dX}{(1-X)^2} = \frac{kC_{A0}^2 V}{F_{A0}}$$

$$V=0 \quad X = X_1 = 0.38$$

$$V = V \quad X = X_2$$

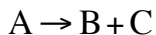
$$\frac{kC_{A0}^2 V}{F_{A0}} = 1 = \frac{1}{1-X_2} - \frac{1}{1-X_1}$$

$$\frac{1}{1-X_2} = 1 + \frac{1}{1-X_1} = 1 + \frac{1}{0.62} = 2.62$$

$$1-X_2 = 0.38$$

$$X_2 = 0.62$$

(25 pts) 10) Study problem P5-9_B. 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 80%.

What is the activation energy in cal/mol?

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

Solution

PFR

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}} = \frac{kC_{A0}(1-X)}{C_{A0}v_0(1+\epsilon X)} = \frac{k(1-X)}{v_0(1+\epsilon X)}$$

$$\int_0^X \frac{(1+\epsilon X)}{(1-X)} dX = \int k \frac{dV}{v_0} = k\tau$$

$$k = \frac{1}{\tau} \left[\left[(1+\epsilon) \ln \frac{1}{1-X} \right] - \epsilon X \right]$$

$$\tau = \frac{10 \text{ dm}^3}{5 \text{ dm}^3/\text{s}} = 2 \text{ s}$$

$$\epsilon = y_{A0}\delta = 1(1+1-1) = 1$$

$$k = \frac{1}{2} \left[(1+1) \ln \left(\frac{1}{1-0.8} \right) - 0.8 \right]$$

$$k = \frac{1}{2} [2 \cdot 1.61 - 0.8] = 1.209 \text{ at } 300\text{K}$$

CSTR

$$V = \frac{F_{A0}X}{-r_A} = \frac{v_0 C_{A0} X}{k C_{A0} \frac{(1-X)}{(1+\epsilon X)}} = \frac{v_0 X (1+\epsilon X)}{k(1-X)}$$

$$\varepsilon = \frac{1}{2}(1+1-1)$$

$$\varepsilon = 0.5$$

$$k = \frac{1}{\tau} \frac{X(1+\varepsilon X)}{(1-X)} = \frac{1}{2} \left[\frac{0.8(1+0.5(0.8))}{0.2} \right]$$

$$= 2.8$$

$$\ln \frac{k_2}{k_1} = \frac{E}{R} \left[\frac{1}{T_1} - \frac{1}{T_2} \right]$$

$$\ln \frac{2.8}{1.21} = \frac{E}{R} \left[\frac{1}{300} - \frac{1}{320} \right] = \frac{E}{R} \frac{20}{(320)(300)}$$

$$E = R \frac{(300)(320)}{20} \ln \frac{2.8}{1.21} \quad , \quad R = 1.987 \frac{\text{cal}}{\text{mol}^\circ\text{K}}$$

$$E = 8010 \frac{\text{cal}}{\text{mol}}$$

