

ChE 344
Fall 2014
Exam I + Solution

Monday, October 20, 2014

Closed Book, Web, Notes, In-Class Problems and Home Problems

Name _____

Honor Code (Please sign in the space provided below)

“I have neither given nor received unauthorized aid on this examination, nor have I concealed any violations of the Honor Code.”

(Signature)

1) ____/ 5 pts

2) ____/ 5 pts

3) ____/ 5 pts

4) ____/ 5 pts

5) ____/ 5 pts

6) ____/ 5 pts

7) ____/10 pts

8) ____/10 pts

9) ____/25 pts

10) ____/25 pts

Total ____/100 pts

Extra Credit:

#) ____/5 pts

ChE 344 - Exam I Cribb Sheet

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. $p = (1 - \alpha w)^{1/2}$

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

$$\frac{dp}{dW} = -\frac{\alpha}{2p} \left(\frac{F_T}{F_{T0}} \right) \left(\frac{T}{T_0} \right), \quad G = \dot{m}/A_C$$

3. Integrals

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

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

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

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

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

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

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

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

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

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

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

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

$$\int_0^X \frac{a + bX}{c + gX} dX = \frac{bX}{g} + \frac{ag - bc}{g^2} \ln \left[\frac{(c + gX)}{c} \right]$$

4. Finite Difference

$$\text{First Point:} \quad -\left. \frac{dC_A}{dt} \right|_{t0} = -\left[\frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t} \right]$$

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

$$\text{e.g.,} \quad -\left. \frac{dC_A}{dt} \right|_{t3} = -\left[\frac{C_{A4} - C_{A2}}{2\Delta t} \right] = \frac{C_{A2} - C_{A4}}{2\Delta t}$$

$$\text{Last Point:} \quad -\left. \frac{dC_A}{dt} \right|_{t5} = -\left[\frac{C_{A3} - 4C_{A4} + 3C_{A5}}{2\Delta t} \right]$$

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.

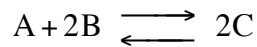
Liquid

1 gal = 3.785 dm³

1 ft³ = 7.482 gal

(5 pts) 1) Chapter 1 Mole Balances

The reaction



takes place in a membrane reactor. The feed is only A and B in equimolar proportions. Which of the following sets of equations gives the correct mole balances on A, B and C?

Species A and B are disappearing and Species C is being formed $\left(-r_A = k_A \left[C_A C_B^2 - \frac{C_C^2}{K_C} \right] \right)$

and C is also diffusing out the sides of a membrane reactor.

Circle the correct answer where all the mole balances are correct

(a)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = r_B$$

$$\frac{dF_C}{dV} = -r_C - R_C$$

Ans: $-r_C$ is wrong

(b)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = 2r_B$$

$$\frac{dF_C}{dV} = 2r_C - 2R_C$$

Ans: $-2R_C$ is wrong

(c)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = r_B$$

$$\frac{dF_C}{dV} = 2r_C - R_C$$

Ans: $2r_C$ is wrong

(d)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = 2r_A$$

$$\frac{dF_C}{dV} = -2r_A - R_C$$

Ans: correct

(e) None of the above

Solution

Answer is (d).

(5 pts) 2) Circle the correct answer.

Consider the following Levenspiel plot for a reversible reaction $A \rightleftharpoons \text{Product}$

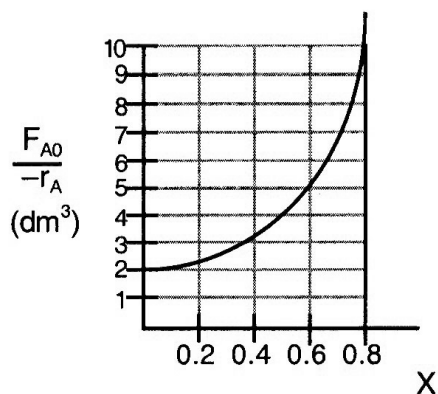
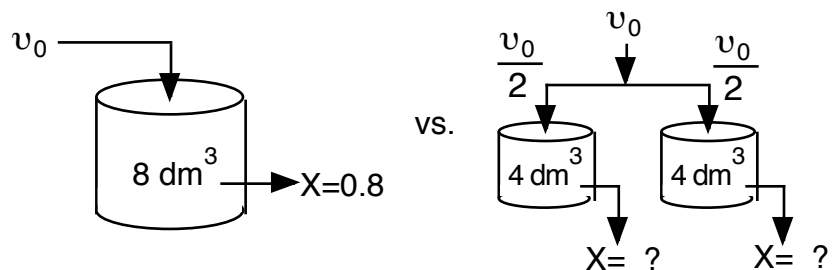


Figure 2-1

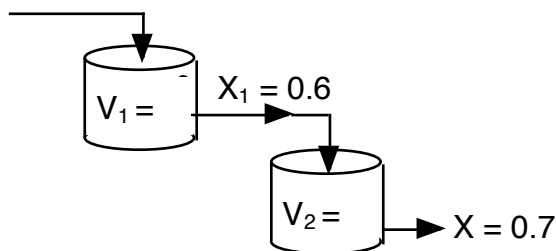
- (1 pt) (a) The equilibrium conversion X_e in a 3 dm^3 reactor is
- (1) $X_e < 0.6$ (2) $X_e = 0.6$ (3) $X_e > 0.6$ (4) Can't tell from the information given
- (2 pt) (b) If the conversion achieved in a single 8 dm^3 CSTR is 80%, what would the conversion be if the flow is equally divided into two CSTRs in parallel with each reactor having a volume of 4 dm^3 each (same total volume).



The total reactor volume is constant at 8 dm^3 .

The conversion for the two reactors in parallel is

- (1) $X > 0.8$ (2) $X < 0.8$ (3) $X = 0.8$ (4) Can't tell from the information given
- (2 pts) (c) What would be the reactor volumes V_1 and V_2 , for two CSTRs connected in series with first reactor having a conversion of 60% and the overall conversion of the second reactor, based on the feed to the first CSTR, is 70%?



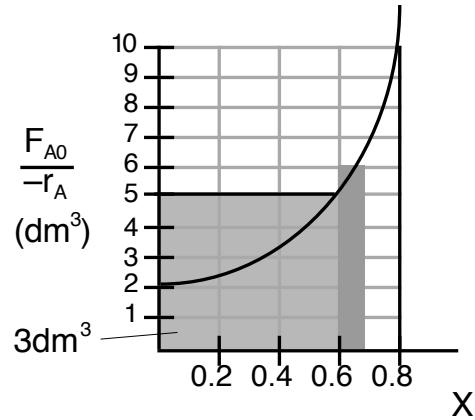
Solution

(a) Ans. (3) $X_e > 0.6$

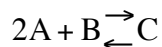
(b) Ans. (3) $X = 0.8$. See p161.

(c) For the first reactor $V_1 = 5 \text{ dm}^3 \times 0.6 = 3 \text{ dm}^3$.

For the $\Delta V = 0.1$ between $X = 0.6$ and 0.7 , $V_2 = 0.1 \times 6 \text{ dm}^3 = 0.6 \text{ dm}^3$



(5 pts) 3) Consider the following reaction



Write the rate law in terms of the specific reaction rate and species concentration when

(1 pt) (a) The reaction is elementary and reversible

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

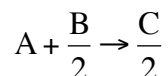
(2 pt) (b) The reaction is irreversible and second order in A, and independent of the concentration of C, and overall first order.

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

(2 pt) (c) Now consider the case when the reaction is irreversible and it is first order in A and first order in B at high concentrations of A and B and is first order in A and second order in B at low concentrations of B. The rate law is

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

Solution

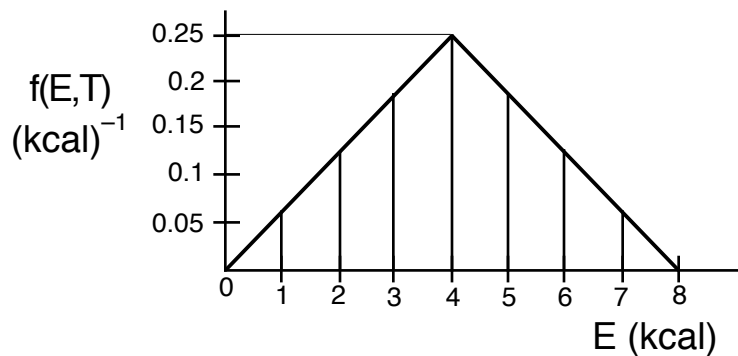


$$(a) \quad -r_A = k_A \left[C_A^2 C_B - \frac{C_C}{K_C} \right]$$

$$(b) \quad -r_A = k_A \frac{C_A^2}{C_B}$$

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

- (5 pts) 4) The following figure shows the energy distribution function at 300 K for the reaction $A + B \rightarrow C$



- (a) What fraction of the collisions have energies between 4 and 5 kcal?
 (b) What fraction of collisions have energies greater than 6 kcal?

Solution

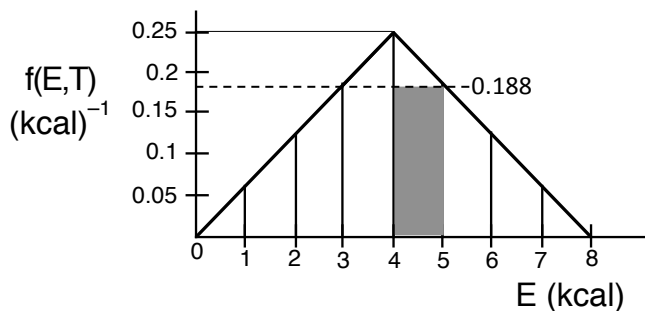
- (a) Between 0 and 4 kcal

$$f(E, T) = \left(\frac{0.25}{4}\right)E$$

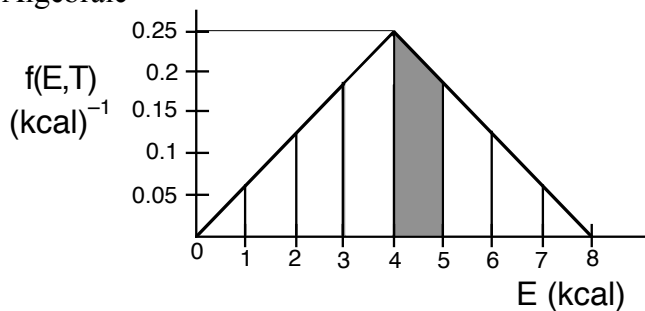
Graphical $(0.25)(1) + 0(0.198)(1) = 0.448$, i.e., 45%

- Between 4 and 8 kcal

$$f(E, T) = 0.5 - \frac{0.25E}{4}$$



Algebraic

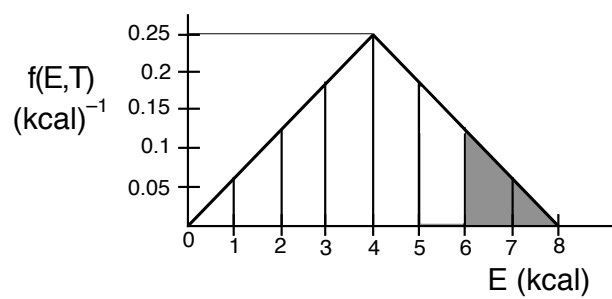


$$\text{at } E = 4, f(E, T) = .25$$

$$\text{at } E = 5, f(E, T) = \frac{3}{4} \cdot .25 = 0.188$$

$$\text{Area} = \left(1 \times (0.25) + (1) \frac{3}{4} \cdot .25\right) / 2 = 22.4\%$$

(b)



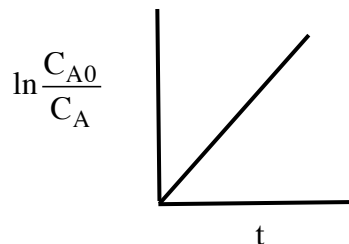
$$F(E, T) = F(6, T) = 0.5 - \frac{0.25}{4} 6 = 0.125$$

$$\text{Area} = \frac{1}{2} (F(6, T) \times 2) = 0.125$$

- (5 pts) 5) Write the rate law for the following plots for the irreversible isothermal isobaric reaction,
 $C_{B0} = 0$.

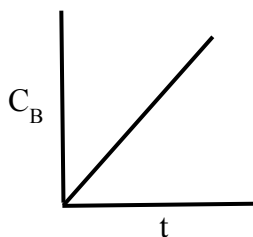


(1 pt) (a)



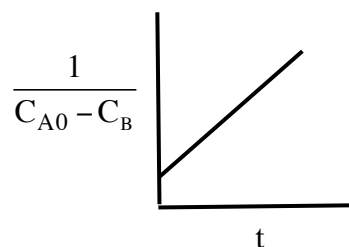
$$-r_A = \underline{\hspace{2cm}}$$

(2 pt) (b)



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

(2 pt) (c)



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

Solution

(a) First order $\frac{dC_A}{dt} = -kC_A$, $t = 0$ $C_A = C_{A0}$

$$\ln \frac{C_{A0}}{C_A} = kt$$

(b) $\frac{dC_A}{dt} = -k$, $\frac{dC_B}{dt} = k$ $t = 0$, $C_B = 0$

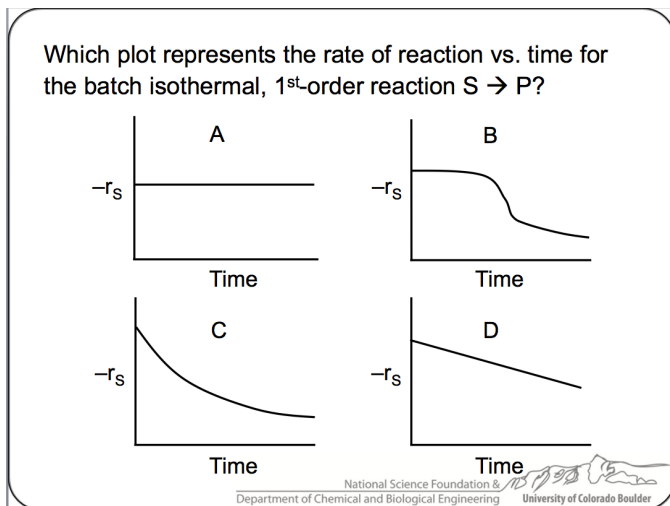
$$C_B = kt \text{ zero order}$$

(c) Second order $\frac{dC_A}{dt} = -kC_A^2$, $t = 0$, $C_A = C_{A0}$

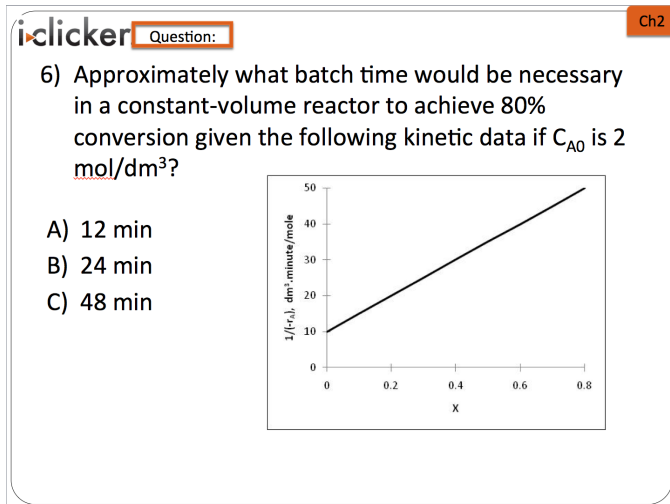
$$kt = \frac{1}{C_A} - \frac{1}{C_{A0}}, C_A = C_{A0} - C_B$$

(5 pts) 6) i>clickers. Circle answers on i>clicker graphs.

(2 pt) (a)

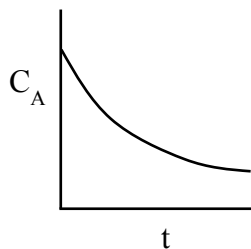


(3 pt) (b)

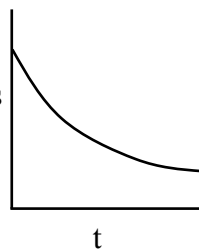


Solution

(a) $-r_s = kC_A$



therefore $-r_s$



(b)

iclicker

Answer:

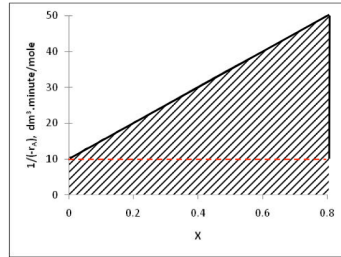
Ch2

6) Approximately what batch time would be necessary in a constant-volume reactor to achieve 80% conversion given the following kinetic data if C_{A0} is 2 mol/dm³?

A) 12 min

B) 24 min

C) 48 min



Solution:

$$t = \int_0^X \frac{C_{A0}}{-r_A} dX = 2 \frac{\text{mol}}{\text{dm}^3} \left[(50 - 10) \times 0.8 \times \frac{1}{2} + (10) \times 0.8 \right] \frac{\text{dm}^3 \cdot \text{min}}{\text{mol}} = 2 [16 + 8] = 48 \text{ minutes}$$

(10 pts) 7) Study Problem 4-4.

P4-4_B Stoichiometry. The elementary gas reaction



is carried out isothermally in a PFR with no pressure drop. The feed is equal molar in A and B and the entering concentration of A is 0.1 mol/dm^3 .

(1 pt) (a) What is the entering concentration (mol/dm^3) of B?

$$C_{B0} = \underline{\hspace{2cm}}$$

(2 pt) (b) What are the concentrations of A and C (mol/dm^3) at 25% conversion of A?

$$C_A = \underline{\hspace{2cm}} \quad C_C = \underline{\hspace{2cm}}$$

(2 pt) (c) What is the concentration of B (mol/dm^3) at 25% conversion of A?

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

(2 pt) (d) If at a particular conversion the rate of formation of C is 2 mol/min/dm^3 , what is the rate of formation of A at the same conversion?

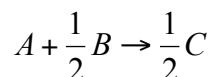
$$r_A = \underline{\hspace{2cm}}$$

(3 pt) (e) Write $-r_A$ solely as a function of conversion (i.e., evaluating all symbols) when the reaction is an elementary, irreversible, gas phase, isothermal reaction with no pressure drop with an equal molar feed and with $C_{A0} = 2.0 \text{ mol/dm}^3$ at, $k_A = 2 \text{ dm}^6/\text{mol}\cdot\text{s}$ to find the rate at $X = 0.25$.

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

Solution

P4-4



$$\varepsilon = y_{A0}\delta = \left(\frac{1}{2}\right)\left[\frac{1}{2} - \frac{1}{2} - 1\right] = -\frac{1}{2}$$

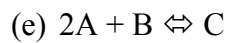
$$(a) \quad C_{B0} = C_{A0} = 0.1 \frac{\text{mol}}{\text{dm}^3}$$

$$(b) \quad C_A = C_{A0} \frac{(1-X)}{(1+\varepsilon X)} = (0.1) \frac{(1-0.25)}{\left(1-\frac{1}{2}X\right)} = \frac{(0.1)(0.75)}{0.875} = 0.086 \frac{\text{mol}}{\text{dm}^3}$$

$$C_C = C_{A0} \frac{\left(\frac{X}{2}\right)}{(1+\varepsilon X)} = (0.1) \frac{\left(\frac{0.25}{2}\right)}{\left(1-\frac{1}{2}X\right)} = \frac{(0.1)(0.125)}{0.875} = 0.0143 \frac{\text{mol}}{\text{dm}^3}$$

$$(c) \quad C_B = C_{A0} = \frac{\left(1 - \frac{1}{2}X\right)}{(1 + \varepsilon X)} = \frac{C_{A0} \left(1 - \frac{1}{2}X\right)}{\left(1 - \frac{1}{2}X\right)} = C_{A0} = 0.1 \frac{\text{mol}}{\text{dm}^3}$$

$$(d) \quad \frac{r_A}{-4} = \frac{r_C}{2}, \quad r_A = -2r_C = -4 \text{ mol/dm}^3/\text{min}$$



$$\varepsilon = \delta y_{A0} = -0.5$$

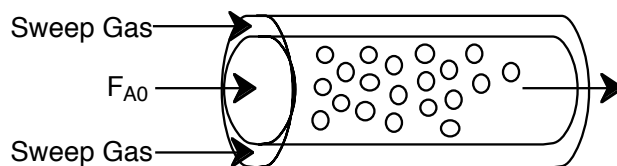
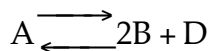
$$C_{A0} = 2 \text{ mol/dm}^3$$

$$-r_A = k(C_A^2 C_B - C_C/K_C)$$

Hence

$$-r_A = 2 \left[4 \left(\frac{1-X}{1-0.5X} \right)^3 - \frac{1}{K_C} \left(\frac{X}{1-0.5X} \right) \right]$$

- (10 pts) 8) The following elementary reaction is carried out in a membrane reactor packed with 100 kg of catalyst. The reaction is carried out isothermally and there is no pressure drop.



The following is a sketch of the concentration profile in a conventional PBR

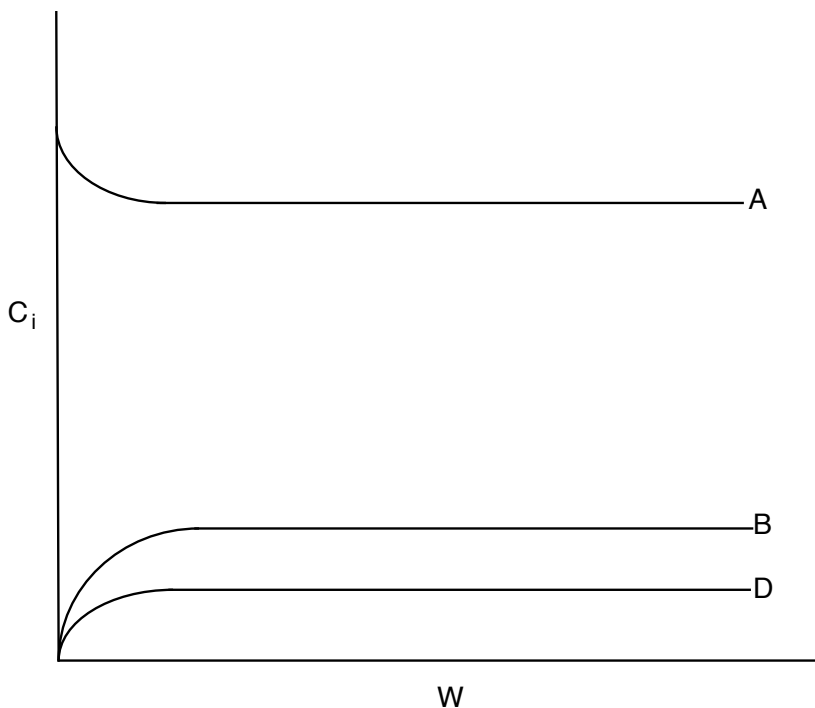
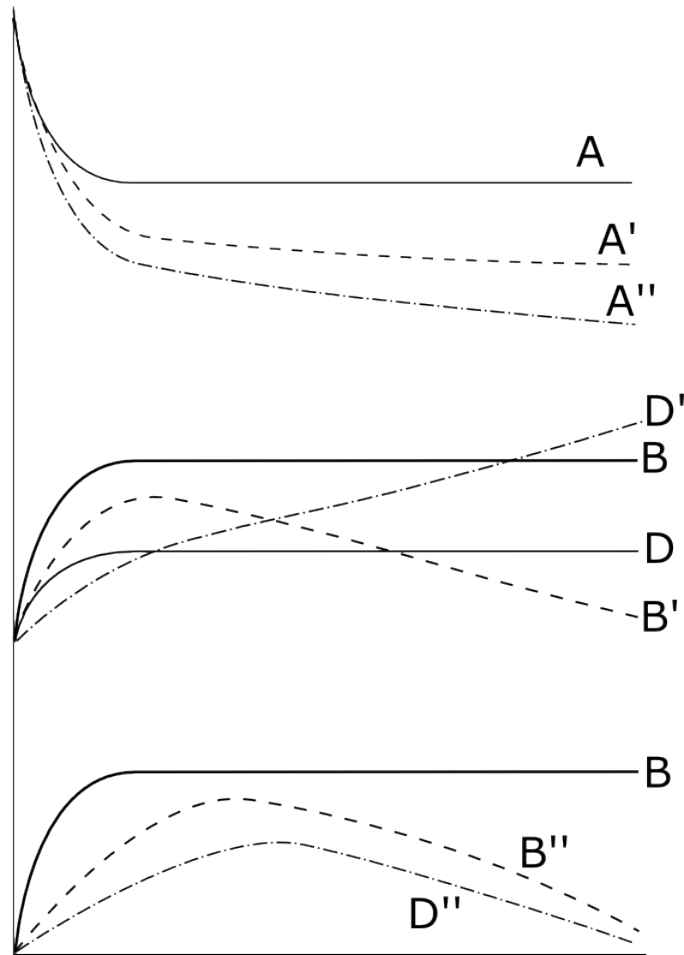


Figure 8-1

- (a) Suppose B diffuses out through the membrane. Using a dashed line (-----) sketch and label the concentration profiles for A, B, and D in a membrane reactor for a moderate value of the mass transfer coefficient for B, k_{CB} , on Figure 8-1. Why?

- (b) Now suppose that both B and D can diffuse out of the reactor. Use a solid line (—) to sketch and label the profiles of A, B, and D on Figure E9-1. Assume the mass transfer coefficients of B and D are the same, $k_{CB} = k_{CD}$. Why?

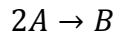
Solution



- (a) The traces are shown in Figure 1, represented by the dotted lines and A', B', and D'. Final concentrations A', and B' will be lower than PBR, while D' will be greater.
- (b) The traces are shown in Figure 1, represented by the solid lines and A'', B'', and D''. Final concentrations A'', B'', and D'' will all be lower than in a PBR. Final concentrations A'' and B'' are lower than final concentrations A' and B'.

$$C_A = C_{T0} \frac{F_A}{F_T} = C_{T0} \frac{F_A}{F_A + F_B + F_C}$$

(25 pts) 9) The elementary irreversible gas phase reaction



is carried out in a constant volume batch reactor where 50 % conversion is achieved in 1 hour. Pure A was charged to the reactor at an initial concentration of 0.2 mol/dm^3 . If the same reaction is carried out in a CSTR, what volume would be necessary to achieve 50 % conversion for a feed molar flow rate of 500 mol/h and an entering concentration of A of 0.2 mol/dm^3 .

$$V_{\text{CSTR}} = \text{_____} \text{ dm}^3$$

Solution

Batch:

$$\frac{dN_A}{dt} = r_A V$$

$$\frac{dX}{dt} = \frac{-r_A}{C_{A0}} = k_A C_{A0} (1-X)^2$$

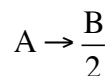
$$\frac{X}{1-X} = k C_{A0} t$$

$$k = \frac{1}{C_{A0} t} \times \frac{X}{1-X} = \frac{1}{0.2 \times 1} \times \frac{0.5}{0.5}$$

$$k = 5 \frac{\text{dm}^3}{\text{mol}}$$

CSTR:

$$V = \frac{F_{A0} X}{-r_A} = \frac{F_{A0} X}{k C_{A0}^2 \left(\frac{1-X}{1+\epsilon X} \right)^2} = \left(\frac{500}{5 \times 0.2^2} \right) \left(\frac{X(1+\epsilon X)^2}{(1-X)^2} \right)$$

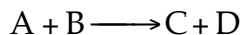


$$\epsilon = y_{A0} \delta = (1) \left(\frac{1}{2} - 1 \right) = -\frac{1}{2}$$

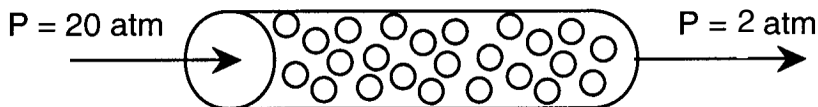
$$V = \frac{500(0.5)(1-0.5 \times 0.5)^2}{(0.2)(1-0.5)^2} = \frac{250(0.75)^2}{(0.2)(0.5)^2}$$

$$V = 2,812.5 \text{ dm}^3$$

(25 pts) 10) The irreversible elementary gas phase reaction



is carried out isothermally at 300 K in a packed bed reactor with 100 kg of catalyst.



The entering pressure was 20 atm and the exit pressure is 2 atm. The feed is equal molar in A and B and the flow is in the turbulent flow regime, with $F_{A0} = 10 \text{ mol/min}$ and $C_{A0} = 0.4 \text{ mol/dm}^3$. Currently 80% conversion is achieved. If the specific reaction rate at 400 K is

$\left[25 \frac{\text{dm}^6}{\text{kgcat} \cdot \text{mol} \cdot \text{min}} \right]$ what is the activation energy?

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

Solution

$$\frac{dX}{dW} = \frac{-r'_A}{F_{A0}} = \frac{kC_{A0}^2(1-X)^2 p^2}{F_{A0}} = \frac{kC_{A0}^2(1-X)^2(1-\alpha W)}{F_{A0}}$$

$$\frac{X}{1-X} = \frac{kC_{A0}^2}{F_{A0}} \left[W - \frac{\alpha W^2}{2} \right]$$

$$p = \frac{2}{20} = 0.1$$

$$p^2 = (1 - \alpha W)$$

$$\alpha = \frac{1-p^2}{W} = \frac{1-0.01}{100} = \frac{0.99}{100}$$

$$\boxed{\alpha = 9.9 \times 10^{-3} \text{ kg}^{-1}}$$

$$\frac{0.8}{1-0.8} = \frac{k \left[0.4 \frac{\text{mol}}{\text{dm}^3} \right]^2}{10 \frac{\text{mol}}{\text{min}}} \left[100 - \frac{(9.9 \times 10^{-3} \times 10^4)}{2} \text{ kg} \right]$$

$$4 = k[0.16][100 - 49.5]/10$$

$$k = 4.95 \frac{\text{dm}^6}{\text{kg mol min}}$$

$$\frac{k(T_2)}{k(T_1)} = e^{\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)}$$

$$\ln \frac{k(T_2)}{k(T_1)} = \frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

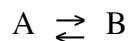
$$\ln \frac{25}{4.95} = \frac{E}{1.987 \frac{\text{cal}}{\text{mol} \cdot \text{K}}} \left(\frac{1}{300} - \frac{1}{400} \right) = \frac{E}{1.987(400)(300)}$$

$$E = 1.987 \frac{(300)(400)}{100} \ln \frac{25}{4.95}$$

$$= 3861 \frac{\text{cal}}{\text{mol}}$$

Extra Credit:

(5 pts) #) For elementary reaction



where Pure A is fed to a reactor the equilibrium conversion is 0.8 at 127°C and 0.5 at 227°C.
What is the heat of reaction?

$$\Delta H_{Rx} = \text{_____ cal/mole A}$$

Solution

$$\frac{X_e}{1 - X_e} = K_C$$

At 127°C, $T_1 = 400 \text{ K}$

$$\frac{0.8}{1 - 0.8} = 4 = K_C$$

At 227°C, $T_2 = 500 \text{ K}$

$$\frac{0.5}{0.5} = 1 = K_C$$

$$\ln \frac{K_{C1}}{K_{C2}} = \frac{\Delta H_{Rx}}{R} \left[\frac{1}{T_1} - \frac{1}{T_2} \right] = \frac{\Delta H_{Rx}}{R} \left[\frac{T_2 - T_1}{T_1 T_2} \right]$$

$$\begin{aligned} \Delta H_{Rx} &= \frac{T_1 T_2}{(T_2 - T_1)} R \ln \frac{K_{C1}}{K_{C2}} \\ &= \frac{(500)(400)}{500 - 400} 1.987 \ln \frac{1}{4} \\ &= (2,000 \text{ K}) 1.987 \frac{\text{cal}}{\text{molK}} (-1.39) \\ &= -5,509 \frac{\text{cal}}{\text{molA}} \end{aligned}$$

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