

(0905421) Chemical Reaction Engineering I

In-Class Assessment # 3 (Chapter 1)

Partner (1) Name: محمد عبد الله Partner (2) Name: محمد عبد الله

Identity (1) #: 0153646

Identity (2) #: 0155794

Self-Test – What Have You Learned?

- Which equation is used in arriving at the design equation for a batch reactor?
☒ a. $G_j = V \cdot r_j$ b. $dN_j/dt = 0$ ☒ c. $F_{j0} = F_j = 0$ d. $E = mc^2$
- What assumptions are made when modeling an ideal tubular reactor? $\rightarrow$ PFR
☒ a. Steady state and no radial variations c. Gas flow and steady state
 b. Plug flow and liquid systems d. That the reactor will photograph well
- What does the mole balance for a CSTR become if $r_j = -k C_j$?
 a. $C_j = (F_{j0} - F_j)/V$ ☒ c. $V = (F_{j0} - F_j)/(k \cdot C_j)$
 b. too complicated d. $V = (F_{j0} - F_j)/k$
- What is the name for any chemical compound or element with a given identity?
 a. Ion b. Atom c. Alfred ☒ d. Chemical species
- Which of the following is a combination type reaction?
 a. 53 left: 37 right: 5 left ☒ b. $A + B \rightarrow C$ c. $A_2 \rightarrow 2A$ d. $A \rightarrow B$
- What happens during a combination reaction?
 a. A molecule breaks down into smaller molecules
 b. You get a burger, fries and a soft drink
☒ c. Two or molecules combine
 d. Species' molecular configuration changes only
- What happens during a decomposition reaction?
 a. Species' molecular configuration changes only
 b. A molecule rots
 c. Two molecules combine to give one molecule
☒ d. A molecule breaks down into smaller molecules
- What assumption is made when studying an IDEAL CSTR?
 a. Innocent until proven guilty ☒ c. Perfect mixing
 b. Adiabatic operation d. Constant volume
- Which of the following reactors usually have the easiest temperature control?
 a. Blue reactors ☒ b. CSTRs c. Tubular reactors d. Batch reactors
const. temp. at all rxn
- A packed bed reactor is also known as a fluidized bed reactor. $\Rightarrow$ CSTR *سواء*
 a. Only when using an alias b. Depends on the catalyst used c. True ☒ d. Always false
- What type of mathematical equation is used to express the rate law?
 a. Irreversible equation c. Unsolvable equation
 b. Differential equation ☒ d. Algebraic equation
- What are the dimensions of k in the equation $-r_A = k C_A$?
 a. moles²/volume²/time c. three
 b. time/mole/volume ☒ d. 1/time

What is Wrong with This Solution?

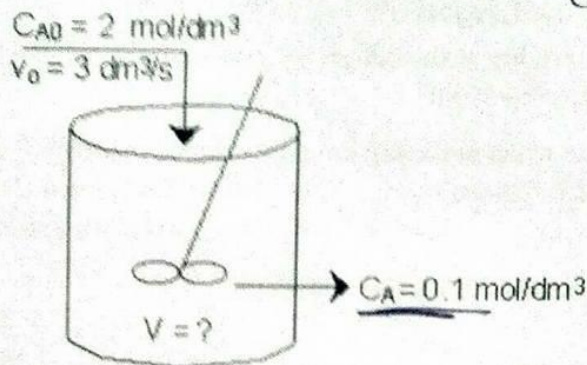
Problem

The irreversible liquid phase second order reaction $2A \xrightarrow{k_1} B$ ($k_1 = 0.03 \text{ dm}^3/\text{mol}\cdot\text{s}$) is carried out in a CSTR. The entering concentration of A, C_{A0} , is 2 M and the exit concentration of A, C_A is 0.1 M. The entering and exiting volumetric flow rate, v_0 , is constant at 3 dm³/s. What is the corresponding reactor volume?

Solution

$$C_{A0} = 2 \text{ M}$$

$$C_{Aout} = 0.1 \text{ M}$$



Mole Balance

$$V = \frac{F_{A0} - F_A}{-r_A}$$

Rate Law

$$-r_A = kC_A^2 \text{ (2nd order)}$$

Combine

$$V = \frac{F_{A0} - F_A}{kC_A^2}$$

$$F_{A0} = v_0 C_{A0} = \frac{3 \text{ dm}^3}{\text{s}} \cdot \frac{2 \text{ mol A}}{\text{dm}^3} = \frac{6 \text{ mol A}}{\text{s}}$$

$$F_A = v_0 C_A = \frac{3 \text{ dm}^3}{\text{s}} \cdot \frac{0.1 \text{ mol A}}{\text{dm}^3} = \frac{0.3 \text{ mol A}}{\text{s}}$$

$$V = \frac{(6 - 0.3) \frac{\text{mol}}{\text{s}}}{\left(0.03 \frac{\text{dm}^3}{\text{mol}\cdot\text{s}}\right) \left(2 \frac{\text{mol}}{\text{dm}^3}\right)^2} = \frac{5.7 \text{ dm}^3}{0.12} = 47.5 \text{ dm}^3$$

$C_A = 0.1 \text{ mol/dm}^3$
exist

What is wrong with this solution?

$$V = 19,000 \text{ dm}^3$$

$\Rightarrow \frac{\text{rate}}{\text{rate}}$

outlet $\rightarrow$ inlet

C_{Aout} $\times$

rate $\rightarrow$ input
input $\rightarrow$ outlet
outlet $\rightarrow$ input

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In-Class Assessment # 2 (Chapter 1)

Partner (1) Name: أحمد، زيد Partner (2) Name: أحمد، زيد

Identity (1) #: 0153646 Identity (2) #: 0155794

Self-Test – What Have You Learned?

$$\rightarrow -r_A = k C_A \quad \text{or} \quad -r_A = k C_A^2$$

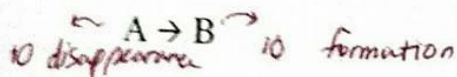
1. The rate law

- (a) is a differential equation ☐ T ☒ F
- (b) relates reaction rate and concentration of reacting species ☒ T ☐ F
- (c) is only valid in the U.S. ☐ T ☒ F
- (d) is a function of temperature; ☒ T ☐ F
and press., conc., catalyst if any

2. The rate of formation of species A is per unit volume is

- (a) r_A ☒ T ☐ F
- (b) $-r_A$ ☐ T ☒ F
- (c) the rate of generation of species A per unit volume ☒ T ☒ F
- (d) r'_A ☐ T ☒ F
- (e) none of the above ☐ T ☒ F

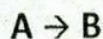
3. Consider the reaction



At a particular time, t , the rate of formation of B in the reaction, r_B , is $10 \text{ mole/dm}^3 \cdot \text{min}$. Which of the following are true?

- (a) The rate of disappearance of B is $-10 \text{ moles/dm}^3 \cdot \text{min}$. ☐ T
- (b) The rate of formation of A is $-10 \text{ mole/dm}^3 \cdot \text{min}$. ☐ T
- (c) The rate of disappearance of A is $10 \text{ moles/dm}^3 \cdot \text{min}$. ☒ T
- (d) $r_A = -10 \text{ moles/dm}^3 \cdot \text{min}$ ☐ T
- (e) $-r_A = 10 \text{ moles/dm}^3 \cdot \text{min}$ ☒ T
- (f) $-r_B = -10 \text{ moles/dm}^3 \cdot \text{min}$ ☐ T
- (g) Some of the above
- ☒ (h) All of the above
- (i) None of the above

Q2: For the reaction



Calculate the time to reduce the number of moles by a factor of 10 ($N_A = \frac{N_{A0}}{10}$) in a batch reactor for the above reaction with $-r_A = kC_A$, when $k = 0.046 \text{ min}^{-1}$

$$N_A = 0.1 N_{A0}$$

$$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$$

~~$$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V} = \frac{N_A - N_{A0}}{r_A V}$$~~

$$= \int_{N_{A0}}^{N_{A0}/10} \frac{dN_A}{-k C_A V} \quad ; \quad \boxed{N_A = C_A V}$$

~~$$= \frac{0.1 N_{A0} - N_{A0}}{r_A V}$$~~

$$= \frac{+1}{k} \int_{N_{A0}/10}^{N_{A0}} \frac{dN_A}{N_A}$$

~~$$t = \frac{-0.9 N_{A0}}{r_A V}$$~~

$$= \frac{1}{k} (\ln N_{A0} - \ln \frac{N_{A0}}{10})$$

~~$$t = \frac{-0.9 C_A}{-k C_A}$$~~

$$= \frac{1}{k} \ln \left(\frac{N_{A0}}{\frac{N_{A0}}{10}} \right)$$

~~$$= \frac{0.9}{0.046}$$~~

$$= \frac{1}{k} \ln (10)$$

~~$$= 19.56$$~~

$$\boxed{t = 50 \text{ min}}$$

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In-Class Assessment # 1 (Chapter 1)

Partner (1) Name: Said, Ali Partner (2) Name: Ali, Ali

Identity (1) #: 0153646 Identity (2) #: 0155794

Q1: Consider the reaction



in which the rate of disappearance of A is 5 moles of A per dm³ per second at the start of the reaction. At the start of the reaction:

(a) What is $-r_A$? 5 mol / dm³.s

(b) What is the rate of formation of B?

$$r_B = -10 \text{ mol / dm}^3 \cdot \text{s}$$

(c) What is the rate of formation of C?

$$r_C = +15 \text{ mol / dm}^3 \cdot \text{s}$$

(d) What is the rate of disappearance of C?

$$-r_C = -15 \text{ mol / dm}^3 \cdot \text{s}$$

(e) What is the rate of formation of A, r_A ?

$$r_A = -5 \text{ mol / dm}^3 \cdot \text{s}$$

(f) What is $-r_B$? rate of disappearance.

$$-r_B = 10 \text{ mol / dm}^3 \cdot \text{s}$$

Levenspiel Plots in Terms of Conversion

For reactions in which the rate depends only on the concentration of one species [i.e., $-r_A = f(C_A)$], it is usually convenient to report $-r_A$ as a function of concentration rather than conversion. We can rewrite the design equation for a plug-flow reactor [Equation (1)] in terms of the concentration, C_A , rather than in terms of conversion for the special case when $[v = v_0]$ isobaric

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

$$F_{A0} = v_0 C_{A0} \quad (2)$$

Now write X in terms of entering and exiting molar flow rate, F_{A0} and F_A :

$$X = \frac{F_{A0} - F_A}{F_{A0}} = \frac{F_{A0} - F_A}{F_{A0}} \quad (3)$$

For the special case when $v = v_0$, plugging Equation (2) into Equation (3), we get

$$X = \frac{F_{A0} - F_A}{F_{A0}} = \frac{C_{A0} v_0 - C_A v_0}{C_{A0} v_0} = \frac{C_{A0} - C_A}{C_{A0}} \quad (4)$$

when $X = 0$, $C_A = C_{A0}$
when $X = X$, $C_A = C_A$

Differentiating Equation (4) yields

$$C_{A0} dX = -dC_A \quad dX = \frac{-dC_A}{C_{A0}} \quad (5)$$

And substituting in Equation (1):

$$V = \frac{F_{A0}}{C_{A0}} \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} \quad (6)$$

Remembering that $\tau = \frac{V}{v_0}$, Equation (6) can be rewritten as:

$$\tau = \frac{V}{v_0} = \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

Equation (7) is a form of the design equation for constant volumetric flow rate v_0 that may prove more useful in determining the space time or reactor volume for reaction rates that depend only on the concentration of one species.

Figure 1 shows a typical curve of the reciprocal reaction rate as a function of concentration for an isothermal reaction carried out at constant volume. For reaction orders greater than zero, the rate decreases as concentration decreases. The area under the curve gives the space time necessary to reduce the concentration of A from C_{A0} to C_{A1} .

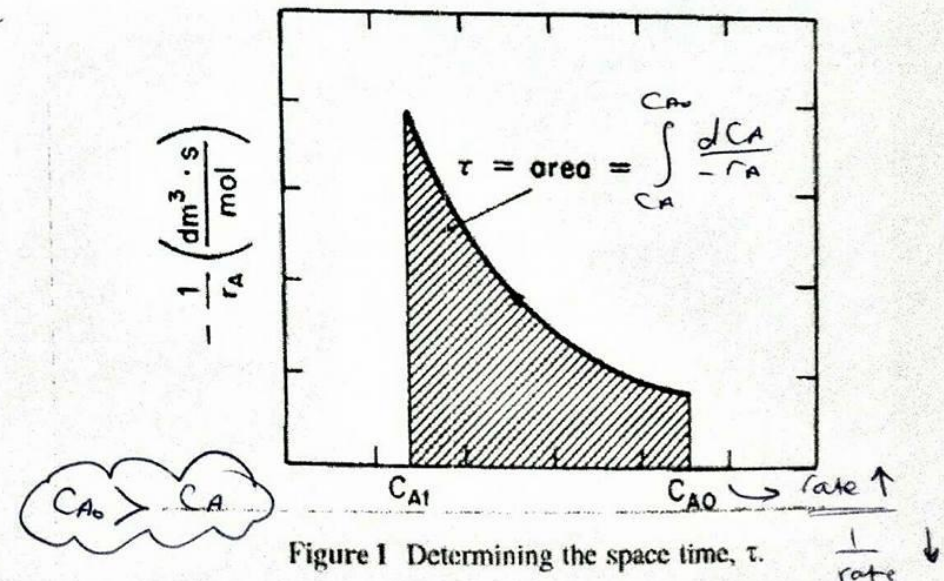
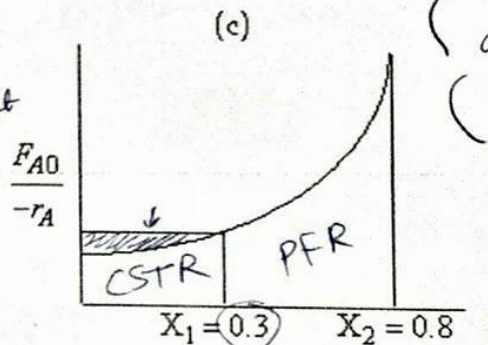
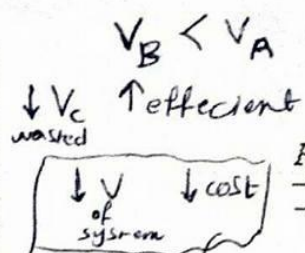
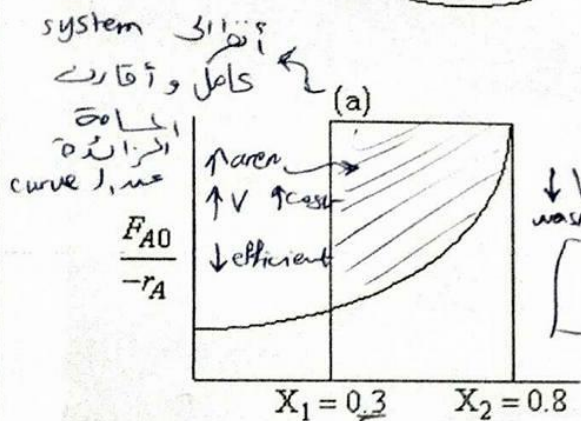
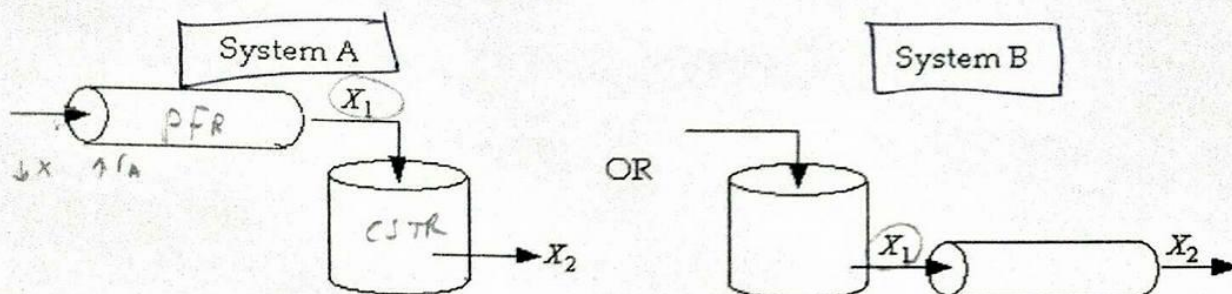


Figure 1 Determining the space time, τ .

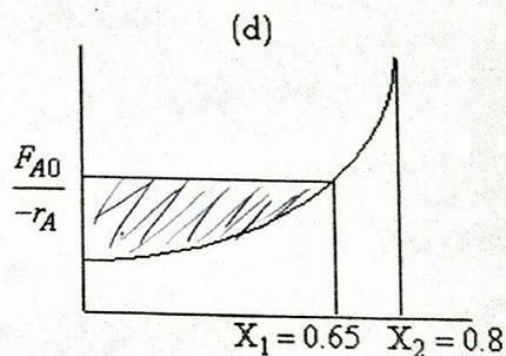
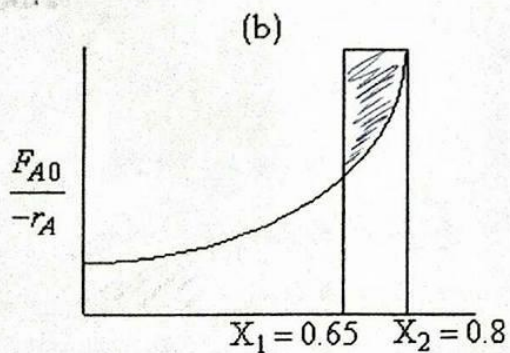
Partner (1) Name: محمد لودي Partner (2) Name: علي علي

Identity (1) #: _____ Identity (2) #: _____

Self-Test



compare
all volume
for all
system.



Q1. Which system is most efficient for an intermediate conversion of (0.3)? B

Q2. Which system is most efficient for an intermediate conversion of (0.65)? **A**

Q3. Which system makes the best use of the reactor volume [i.e., least "wasted" volume]? (C)

describe [C]: CSTR flowed by PFR with intermediate conversion of 0.3.

Partner (1) Name: Sami Al-Jarrah Partner (2) Name: Ali

Identity (1) #: _____ Identity (2) #: _____

The gas-phase reaction $A + B \rightarrow C$ described by the data in the table below is to be carried out at 10 atm and 227 °C. The feed contains 41% A, 41% B, and 18% inert, and flows at a rate of 1 mol/s. $\{A_0$

$-r_A$ (mol/(L.min))	0.2	0.0167	0.00488	0.00286	0.00204
X	0.0	0.1	0.4	0.7	0.9

(a) What is the volume of a single CSTR back-mix reactor necessary to achieve 70% conversion?

$$V = \frac{F_{A_0} X}{-r_A} = \frac{(1) (0.7)}{0.00286} = 244.755 \text{ X units}$$

$$\frac{1 \text{ mol}}{\text{s}} \times \frac{0.7}{0.00286} \times \frac{\text{L.min}}{60 \text{ s}} = 14.686 \text{ L} = 14.700 \text{ m}^3$$

(b) What is the volume of a single PFR tubular reactor necessary to achieve 60% conversion?

$$X=0 \rightarrow \frac{F_{A_0}}{-r_A} = \frac{1}{0.2} = 5 \times 60 = 300 = 0.3 \text{ KL}$$

$$X=0.1 \rightarrow \frac{F_{A_0}}{-r_A} = \frac{1}{0.0167} = 3592.8 = 3.5928$$

$$X=0.4 \rightarrow \frac{F_{A_0}}{-r_A} = \frac{1}{0.00488} = 12295.08 = 12.29508$$

$$X=0.6 \rightarrow \frac{F_{A_0}}{-r_A} = \frac{1}{3.53 \times 10^{-3}} = 283.3 \times 60 = 16998 \text{ L}$$

$$X=0.7 \rightarrow \frac{F_{A_0}}{-r_A} = \frac{1}{0.00286} = 20979 = 20.979$$

$$X=0.9 \rightarrow \frac{F_{A_0}}{-r_A} = \frac{1}{0.00204} = 29411.76 = 29.4118$$

= triangle Area

$$= \frac{1}{2} (0.6) (18,000) (\text{KL})$$

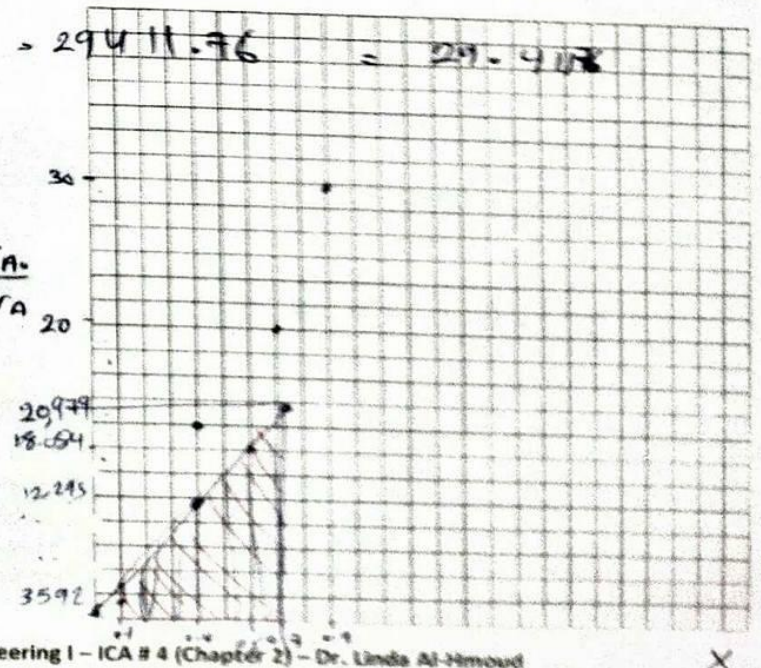
$$= 5400 \text{ L}$$

$$= 5.400 \text{ m}^3$$

$$V = \int_0^X \frac{F_{A_0}}{-r_A} dX$$

0.00353

$$X=0.6 \rightarrow -r_A = 3.53 \times 10^{-3} \frac{\text{mol}}{\text{L.min}}$$



$$X=0 \Rightarrow V = \frac{F_{A0}}{-r_A} = \frac{1}{0.2} \times 60 = 300 \text{ L}$$

$$X=0.1 \Rightarrow V = \frac{F_{A0}}{-r_A} = \frac{1}{0.0167} \times 60 = 3592.8 \text{ L}$$

$$X=0.4 \Rightarrow V = \frac{F_{A0}}{-r_A} = \frac{1}{0.00488} \times 60 = 12,295.08 \text{ L}$$

↓

$$\text{interpolation} \Rightarrow \frac{0.4 - 0.7}{12,295.08 - 20,979} = \frac{0.4 - 0.6}{12,295.08 - X}$$

$$X=0.6 \Rightarrow \frac{F_{A0}}{-r_A} = 18,084 \text{ L}$$

$$X=0.7 \Rightarrow V = \frac{F_{A0}}{-r_A} = \frac{1}{0.00286} \times 60 = 20,979 \text{ L}$$

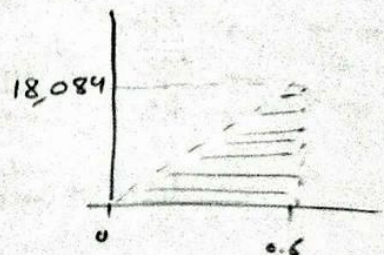
Volume in PFR = area under the curve

$$A = V = \frac{1}{2} (x) \left(\frac{F_{A0}}{-r_A} \right)$$

under the curve

$$= \left(\frac{1}{2} \right) (0.6) (18,084)$$

$$= 5425.2 \text{ L}$$



In-Class Assessment # 5 (Chapter 2)

Partner (1) Name: اسامی علی

Partner (2) Name: WLS, Inc

Identity (1) #: _____

Identity (2) #: _____

A 400-L CSTR and a 100-L PFR are available to process 1.0 L of feed per second. The feed contains 41% A, 41% B, and 18% inert. The irreversible gas-phase reaction $A + B \rightarrow C$ is to be carried out at 10 atm and 227 °C. The rate of reaction in mol/(L.min) is given below as a function of conversion:

$-r_A$	0.2	0.0167	0.00488	0.00286	0.00204
X	0.0	0.1	0.4	0.7	0.9

in the back (a) What is the maximum conversion that can be achieved with these two reactors connected in series?

$$C_{A0} = 0.41 \text{ (10 atm)}$$

$$0.08206 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}} \times (227 + 273) \text{ K} = 0.1 \text{ mol/L}$$

$$F_{A_0} = 0.1 \frac{\text{mol}}{\text{L}} \times 1 \frac{\text{L}}{\text{s}} = 0.1 \text{ mol/s} = 6 \text{ mol/min}$$

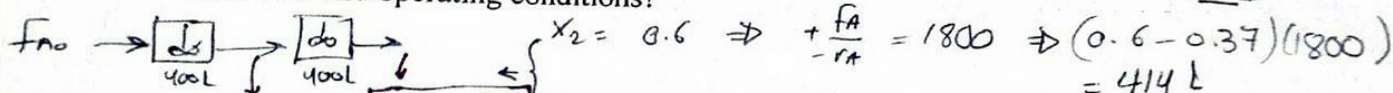
$$P_0 V_0 = F_{T_0} RT = pV = nR\theta$$

$$\frac{f_{T_0}}{\sqrt{V_{T_0}}} = C_{T_0} = \frac{P_{T_0}}{R T_0}$$

$$C_{A0} = \frac{y_{A0} P_0}{R T_0}$$

$$X = \frac{V \cdot \Delta}{F_0} =$$

(b) What would be the overall conversion if two 400-L CSTRs were connected in series for the same feed and operating conditions?

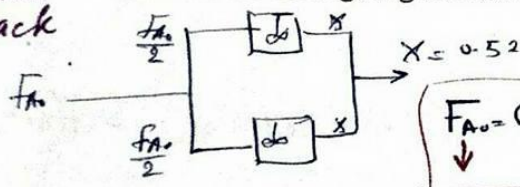


$$X_1 = 0.37 \quad \boxed{X_2 = 0.59}$$

$$x_2 = 0.5 \Rightarrow \frac{f_A}{-r_A} = 1580 \Rightarrow (0.5 - 0.37)(1580)$$

(c) What would be the overall conversion if two 400-L CSTRs were connected in parallel with half of the feed going to each reactor? $p\gamma = F_A \cdot R_T$

$$pV = F_A \cdot RT$$



$$\left(\begin{array}{c} F_{Au} = G_{Au} \cdot \Delta u \\ \downarrow \qquad \downarrow \end{array} \right) \Rightarrow \left(\begin{array}{c} \uparrow \\ \downarrow \end{array} \right) I = \frac{V}{\Delta u}$$

$$\Rightarrow \boxed{Z \uparrow \Rightarrow X \uparrow}$$

the conversion
will be increase

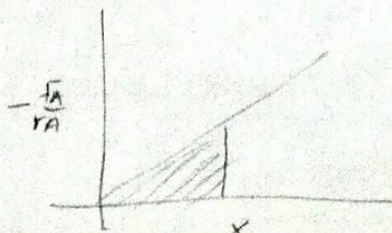
(d) If the total pressure were reduced by a factor of 10, would the conversion increase, decrease, or remain the same? *continuous system* X

$$P_2 = 0.1 P_1$$

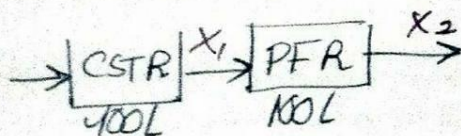
$$P_r = FRT$$

$\downarrow P \uparrow \nu \Rightarrow \uparrow \nu \downarrow \lambda \downarrow x \Rightarrow$ the conversion will be decrease

(e) Plot the rate of reaction and conversion as a function of PFR volume



⑨ case ①



* for CSTR:

$$X = 0.3 \Rightarrow \frac{F_A}{-r_A} = 800$$

$$\Rightarrow 0.3 \times 800 = 240 \text{ L}$$

Interpolation

$$X = 0.366$$

$$X_1 = 0.37$$

* for PFR:

$$X = 0.45 \Rightarrow \frac{F_A}{-r_A} = 1250$$

$$\Rightarrow \frac{(0.45 - 0.4)(1250) + \frac{1}{2}(0.45 - 0.4)(1400 - 1250)}{0.05} = 65 \text{ L}$$

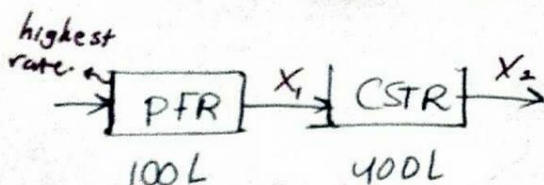
Interpolation

$$X_2 = 0.48$$

$$X = 0.50 \Rightarrow \frac{F_A}{-r_A} = 1400$$

$$\Rightarrow (0.5 - 0.4)(1250) + \frac{1}{2}(0.5 - 0.4)(1600 - 1250) = 120 + 15 = 135 \text{ L}$$

Case ②



* for PFR:

$$X_1 = 0.2 \Rightarrow \frac{F_A}{-r_A} = 600 \Rightarrow \frac{1}{2} \times 0.2 \times 600 = 60 \text{ L}$$

$$= 0.3 \Rightarrow \frac{F_A}{-r_A} = 580 \Rightarrow \frac{1}{2} \times 0.3 \times 900 = 135 \text{ L}$$

$$X_1 = 0.25$$

* for CSTR:

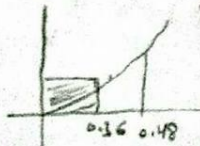
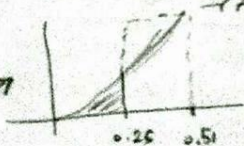
$$X_2 = 0.5 \Rightarrow \frac{F_A}{-r_A} = 1500 \Rightarrow (0.5 - 0.25) \times 1500 = 375 \text{ L}$$

$$X_2 = 0.6 \Rightarrow \frac{F_A}{-r_A} = 1800 \Rightarrow (0.6 - 0.25) \times 1410 = 630 \text{ L}$$

$$X_2 = 0.509$$

$$X_2 = 0.51$$

the best.



the case ② better than case ①

⑩ $X = 0.5$, $\frac{F_A}{-r_A} = 750 \Rightarrow 0.5 \times 750 = 375 \text{ L}$

$$X = 0.55, \frac{F_A}{-r_A} = 790 \Rightarrow 0.55 \times 790 = 434.5$$

$$X = 0.52$$

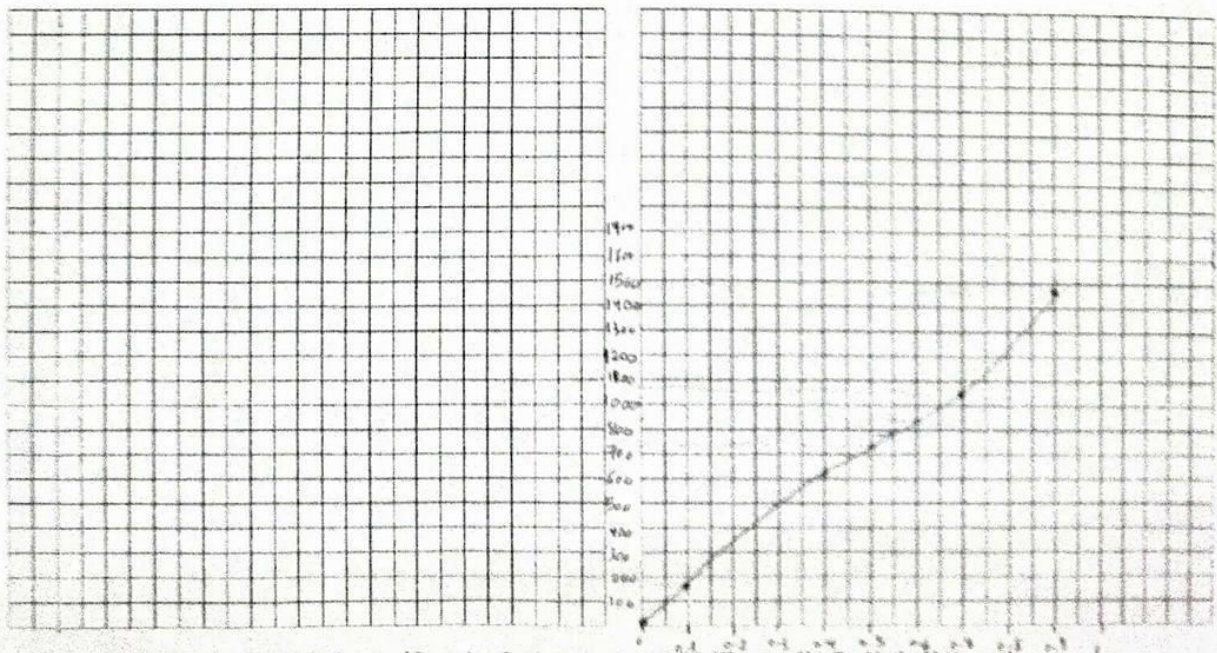
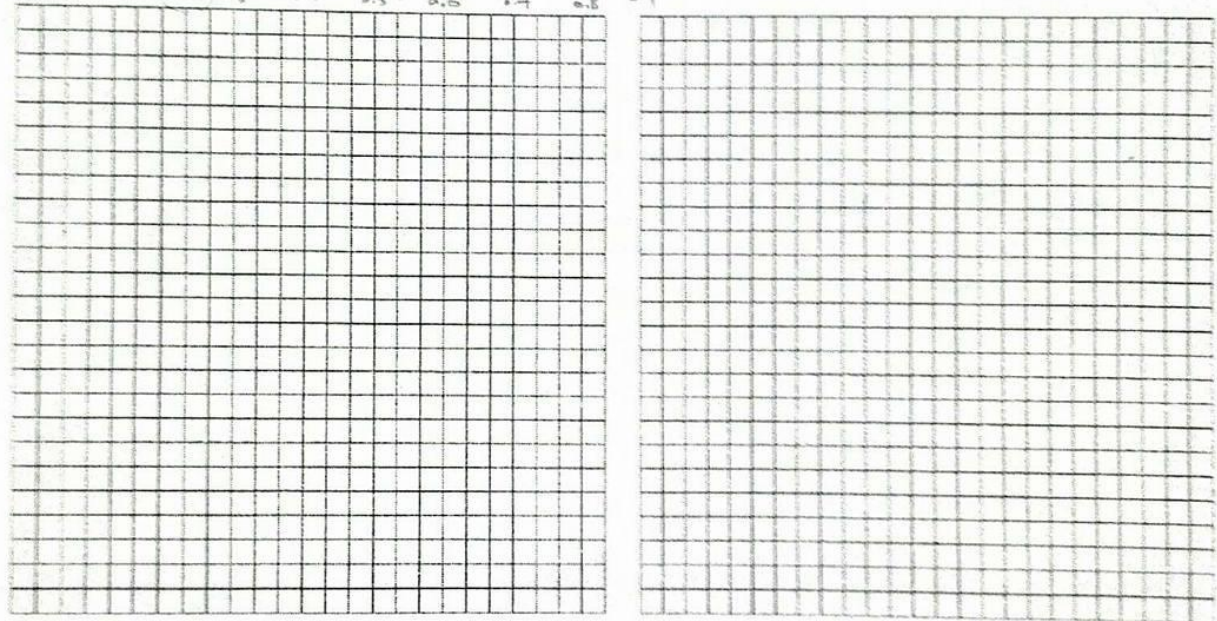
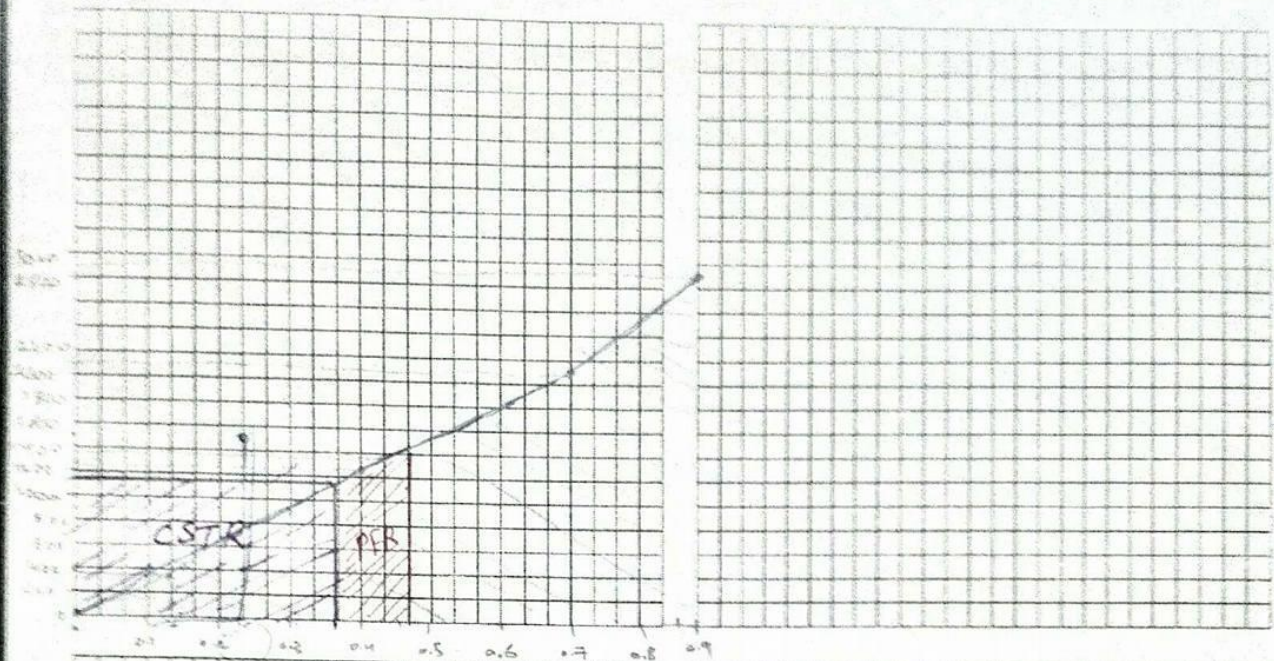
$$X_c = 0.2 \rightarrow \frac{F_{A0}}{V} = 480 \rightarrow V = 0.2 \times 480 = 96 \text{ L}$$

$$X_c = 0.4 \rightarrow -r_A$$

$$V = 500 \text{ L}$$

$$X_c = 0.37 \Rightarrow V = 360 \text{ L}$$

$$X_c = 0.42 \Rightarrow V = 100 \text{ L}$$



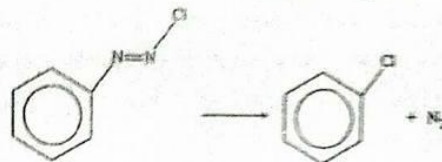
(0905421) Chemical Reaction Engineering I

In-Class Assessment # 10 (Chapter 3)

Partner (1) Name: Sy W. Al-Haj Partner (2) Name: Sy W. Al-Haj

Identity (1) #: 0153646 Identity (2) #: 0153646

Using the data in the table below, calculate the activation energy for the first order decomposition of benzene diazonium chloride to give chlorobenzene and nitrogen:



$k \rightarrow A e^{-\frac{E_a}{RT}}$
for (Temp)
independent

$k(s^{-1})$	0.00043	0.00103	0.00180	0.00355	0.00717
$T(K)$	313.0	319.0	323.0	328.0	333.0
$\ln k$	-7.75	-6.88	-6.32	-5.64	-4.94
$1/T$	3.2×10^{-3}	3.14×10^{-3}	3.1×10^{-3}	3.05×10^{-3}	3×10^{-3}

$\times 10^{-3} (1/T)$ $\ln(k)$

3.1	-6.5
3.15	-7.20

$\times 10^{-3} (1/T)$ $\ln(k)$

3.16	-7.20
3.06	-5.8

slope = $-\frac{E}{R}$
slope = -14

(2.0) $\ln A$ intercept
activation energy
from slope

slope = $\frac{-7.20 + 6.5}{3.15 - 3.1}$

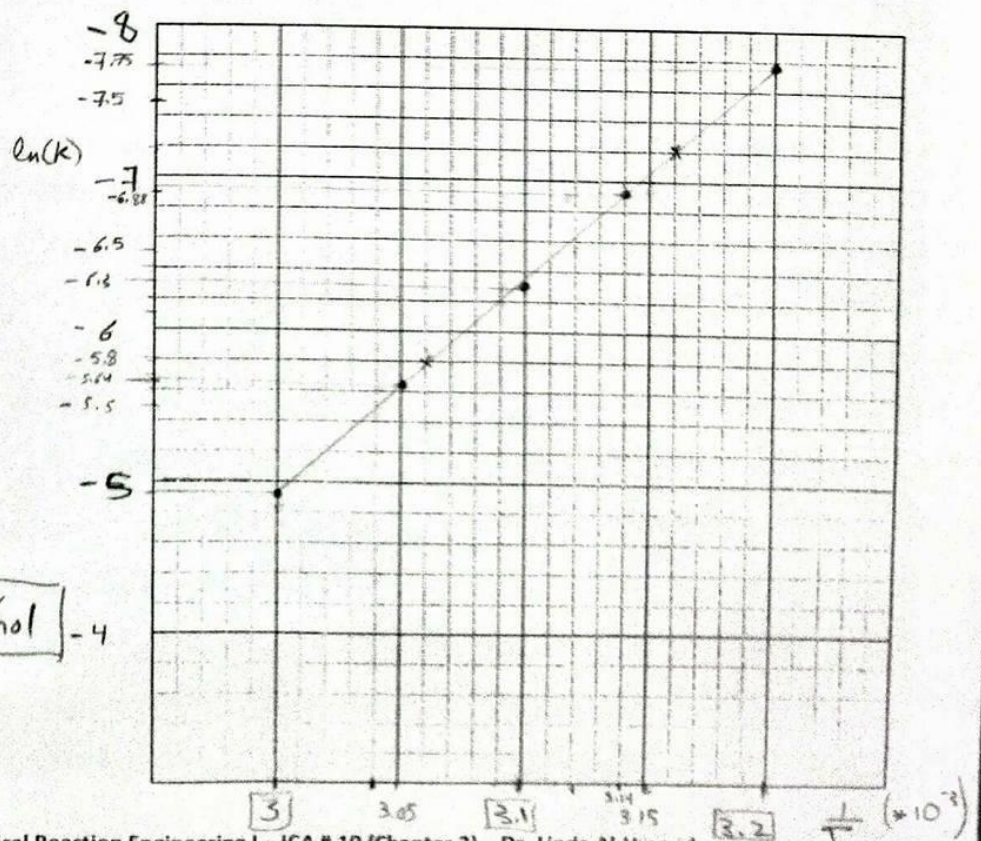
slope = -14

$-14 = -\frac{E}{R}$

$-14 = \frac{-E}{8.314}$

$E = 14 \times 8.314$

$E = 116.396 \text{ kJ/mol}$

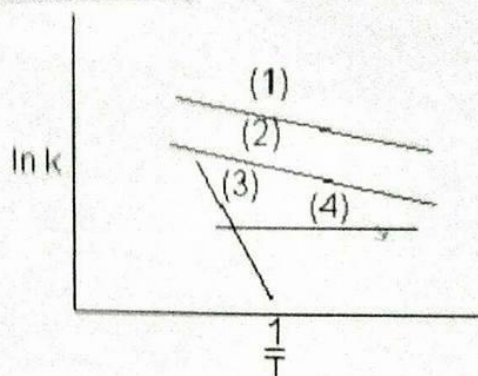
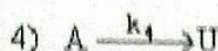
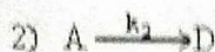


Pop Quiz # 1 (Chapter 3)

Name: Ali H. Al-Hmoud

ID # 0152646

Consider the following elementary reactions



$$\ln k_A = \ln A - \frac{E_a}{R} \left(\frac{1}{T} \right)$$

↑ slope ↑ E

slope = 0 $\propto$ E_a independent on temp.

1) Which reaction is virtually temperature insensitive?

(1) (2) (3) **(4)**

2) Which reactions have the same activation energy?

→ Same slope

1 AND **2**

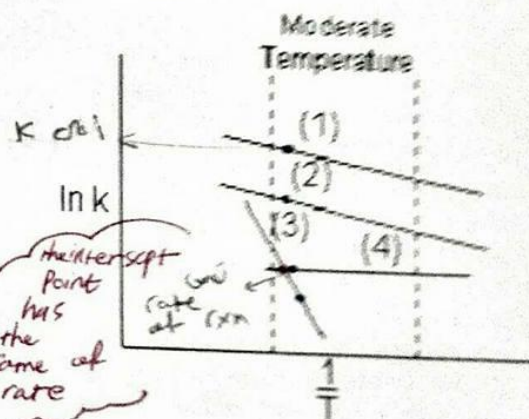
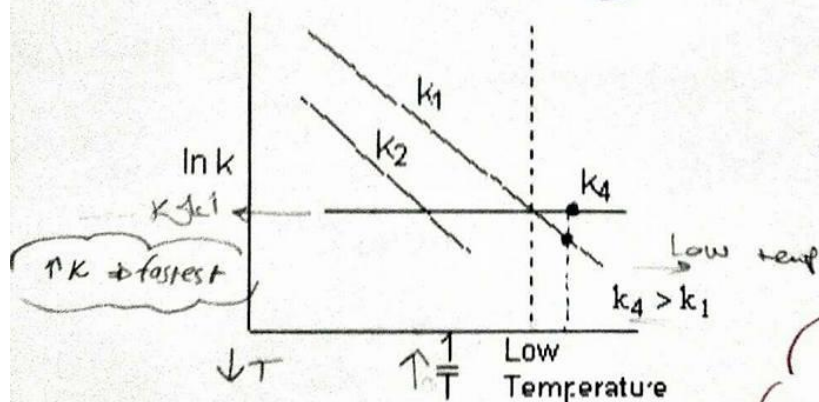
3) Which reaction will dominate (i.e. take place the fastest) at

(a) low temperatures?

(1) (2) (3) **(4)**

(b) moderate temperatures?

(1) (2) (3) (4)

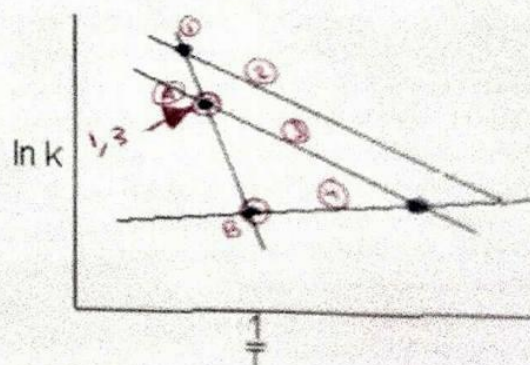


4) Label 2 intersecting points and complete the following sentences:

same rate of rxn

1- At point A, reaction 1 and reaction 3 will have the same rate of reaction at a given temperature.

2- At point B, reaction 1 and reaction 4 will have the same rate of reaction at a given temperature.



⇒ assume NH_3 is the limiting reactant.

(3) $\boxed{\text{NH}_3 = A}$



Species	Symbol	Initial	Change	Remaining
NH_3	A	N_{A0}	$-N_{A0} X$	$N_{A0}(1-X)$
O_2	B	$N_{B0} = N_{A0} \theta_B$	$-\frac{5}{4} N_{A0} X$	$N_{A0}(\theta_B - \frac{5}{4} X)$
NO	C	—	$N_{A0} X$	$N_{A0} X$
H_2O	D	—	$\frac{3}{2} N_{A0} X$	$\frac{3}{2} N_{A0} X$
N_2	I	$N_I = \theta_I N_{A0}$	—	$\theta_I N_{A0}$

inert
جواب نهی
۵، ۳، ۲

$$\theta_B = \frac{C_{B0}}{C_{A0}} = \frac{y_{B0}}{y_{A0}} = \frac{(0.21)(0.85)}{0.15} = 1.2$$

$$\theta_I = \frac{(0.79)(0.85)}{0.15} = 4.5$$

(a)

$$C_A = \frac{N_{A0}}{V_0} = C_{A0}(1-X)$$

$$C_B = C_{A0}(\theta_B - \frac{5}{4}X)$$

$$C_C = C_{A0}X$$

$$C_I = C_{A0}\theta_I$$

$$C_D = \frac{3}{2} C_{A0}X$$

$$C_T = C_{A0} + C_{A0}\theta_B - \frac{5}{4}C_{A0}X + \frac{3}{2}C_{A0}X + \theta_I C_{A0}$$

$$= C_{T0} + \left(\frac{1}{4}\right)C_{A0}X$$

$1 + \frac{3}{2} - 1 - \frac{5}{4} = \frac{1}{4}$

$$P_T = C_T R T_0$$

$$P_T = (C_{T0} + \frac{1}{4}C_{A0}X) R T_0 \quad ; C_{A0} = 0.03 \text{ mol/L}$$

$$P_T = (0.2 + \frac{1}{4}(0.03)X) (6.08206 \times 500)$$

$$P_T = (0.2 + 7.5 \times 10^{-2} X) (41.03)$$

(0905421) Chemical Reaction Engineering I

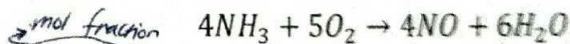
In-Class Assessment # 9 (Chapter 3)

Partner (1) Name: س. م. ع. ع. ع. Partner (2) Name: م. م. ع. ع. ع.

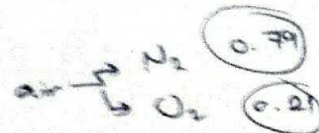
Identity (1) #: _____ Identity (2) #: _____

Production of Nitric acid

Nitric acid is made commercially from nitric oxide. Nitric oxide is produced by the gas-phase oxidation of ammonia.



The feed consists of 15 mol% ammonia in air at 8.2 atm and 227 °C.



- What is the total entering concentration?
- What is the entering concentration of ammonia?
- Set up a stoichiometric table with ammonia as your basis of calculation. constant-volume batch reactor.
 - Express C_i for all species as functions of conversion for a constant-volume batch reactor. Express P_T as a function of X .
 - Express P_i and C_i for all species as functions of conversion for a flow reactor. $\rightarrow$ gas-phase (non. const. volume)
- Write the combined rate law solely in terms of the molar flow rates and rate law parameters for 3(a) and 3(b) above. Assume the reaction is first order in both reactants and the specific reaction rate at the given condition is 5000 L/(mol.min). k_1

NH_3	O_2
$\frac{0.15}{4}$	$\frac{0.85 \times 0.21}{5}$
$\boxed{0.0375}$	$\boxed{0.0357}$



$$P = CRT$$

$$8.2 \text{ atm} = C \times (227 + 273)$$

$$C = 0.1998$$

$$C \leq 0.20$$

NH_3 is the limiting reactant

O_2 is the limiting reactant

$$\textcircled{1} C_{T0} = \frac{P_0}{RT_0} = 0.2 \text{ mol/L}$$

$$\textcircled{2} C_{A0} = y_{A0} C_{T0} = 0.15 (0.2) = 0.03 \text{ mol/L}$$

⇒ assume NH_3 is the limiting reactant

(3) $\boxed{\text{NH}_3 = A}$



Species	Symbol	Initial	Change	Remaining
NH_3	A	N_{A0}	$-N_{A0} X$	$N_{A0}(1-X)$
O_2	B	$N_{B0} = N_{A0} \theta_B$	$-\frac{5}{4} N_{A0} X$	$N_{A0}(\theta_B - \frac{5}{4} X)$
NO	C	—	$N_{A0} X$	$N_{A0} X$
H_2O	D	—	$\frac{3}{2} N_{A0} X$	$\frac{3}{2} N_{A0} X$
N_2	I	$N_I = \theta_I N_{A0}$	—	$\theta_I N_{A0}$

inert
بازمانده
۱, ۳, ۵

$$\theta_B = \frac{C_{B0}}{C_{A0}} = \frac{y_{B0}}{y_{A0}} = \frac{(0.21)(0.85)}{0.15} = 1.2$$

$$\theta_I = \frac{(0.79)(0.85)}{0.15} = 4.5$$

(a)

$$C_A = \frac{N_{A0}}{V_0} = C_{A0}(1-X)$$

$$C_B = C_{A0}(\theta_B - \frac{5}{4}X)$$

$$C_C = C_{A0}X$$

$$C_I = C_{A0}\theta_I$$

$$C_D = \frac{3}{2} C_{A0}X$$

$$C_T = C_{A0} + C_{A0}\theta_B - \frac{5}{4}C_{A0}X + \frac{3}{2}C_{A0}X + \theta_I C_{A0}$$

$$= C_{T0} + \left(\frac{1}{4}\right)C_{A0}X$$

$$1 + \frac{3}{2} - 1 - \frac{5}{4} + \frac{1}{4}$$

$$P_T = C_T R T_0$$

$$P_T = (C_{T0} + \frac{1}{4}C_{A0}X) R T_0 \quad ; \quad C_{A0} = 0.03 \text{ mol/L}$$

$$P_T = (0.2 + \frac{1}{4}(0.03)X) (6.08206 \times 500)$$

$$P_T = (0.2 + 7.5 \times 10^{-3} X) (41.03)$$



3.b

$$C_A = \frac{C_{A0}(1-x)}{(1+\epsilon x)}$$

$\frac{P}{P_0}$ $\frac{T_0}{T}$
 ① ①
 isobaric isothermal

$$P_A = C_A RT \quad T = 500 \text{ K}$$

$$C_B = \frac{C_{A0}(\Theta_B - \frac{5}{4}x)}{(1+\epsilon x)} = \frac{0.03(1.2 - \frac{5}{4}x)}{(1+0.0375)}$$

$$P_B = C_B RT$$

$$C_C = \frac{C_{A0}x}{(1+\epsilon x)}$$

$$P_C = C_C RT$$

$$C_D = \frac{\frac{3}{2}C_{A0}x}{(1+\epsilon x)}$$

$$P_D = C_D RT$$

$$C_I = \frac{C_{A0}\Theta_I}{(1+\epsilon x)}$$

$$P_I = C_I RT$$

$$\epsilon = \nu_{A0} \Delta$$

$$\Delta = 1 + \frac{3}{2} - 1 - \frac{5}{4} = \frac{1}{4}$$

$$\epsilon = (0.15) \left(\frac{1}{4}\right) = 0.0375$$

$$C_{A0} = 0.03 \text{ mol/L}$$

$$\textcircled{4} \quad -r_A = k \underline{C_A} \underline{C_B}$$

$$\text{3(a)} \Rightarrow -r_A = k C_{A0} (1-x) C_{A0} \left(\Theta_B - \frac{5}{4} x \right) \Rightarrow \text{const. volume}$$

$$\text{3(b)} \Rightarrow -r_A = k C_{A0}^2 \frac{(1-x) \left(\Theta_B - \frac{5}{4} x \right)}{(1+\varepsilon x)^2} \Rightarrow \text{NOT const. volume.}$$

(0905421) Chemical Reaction Engineering I

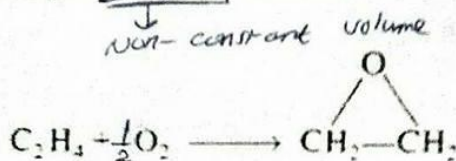
In-Class Assessment # 11 (Chapter 3)

Partner (1) Name: Osman Is Partner (2) Name: Ali Al

Identity (1) #: _____ Identity (2) #: _____

P3-11A Set up a stoichiometric table for each of the following reactions and express the concentration of each species in the reaction as a function of conversion evaluating all constants (e.g. ϵ , Θ). Then, assume the reaction follows an elementary rate law, and write the reaction rate solely as a function of conversion, i.e., $-r_A = f(X)$.

(c) For the isothermal, isobaric, catalytic gas-phase oxidation

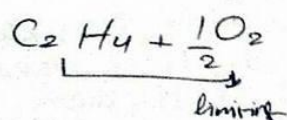


the feed enters a PBR at 6 atm and 260°C and is a stoichiometric mixture of only oxygen and ethylene.

→ NO limiting reactants

$\Theta_B = \frac{1/2}{1} = 1/2$

no limiting
 $\frac{1}{2}\text{O}_2$ & C_2H_4



$\Theta_B = \frac{f_{B0}}{f_{A0} + f_{B0}} = \frac{1}{1+1/2}$
Just from stoichiometric

① Stoich. table

Species	Symbol	Feed	change	effluent
C_2H_4	A	F_{A0}	$-F_{A0}X$	$F_{A0}(1-X)$
O_2	B	$F_{B0} = F_{A0}\Theta_B$	$-\frac{1}{2}F_{A0}X$	$F_{A0}\left(\Theta_B - \frac{1}{2}X\right)$
CH_2OCH_2	C	$F_{C0} = 0$	$+F_{A0}X$	$F_{A0}X$

$\Theta_B = \frac{1}{2}$

$C_A = \frac{F_A}{V} = \frac{F_{A0}(1-X)}{V_0(1+\epsilon X)} = C_{A0} \frac{(1-X)}{(1-\frac{X}{3})}$

$C_B = \frac{C_{A0}}{2} \frac{(1-X)}{(1-\frac{X}{3})}$

$C_C = \frac{C_{A0}X}{(1-\frac{X}{3})}$

$\epsilon = S \Theta_B = (1 - \frac{1}{2} - 1) \left(\frac{1}{1 + \frac{1}{2}} \right)$
 $= -\frac{1}{3}$

(0905421) Chemical Reaction Engineering I – ICA # 11 (Chapter 3) – Dr. Linda Al-Hmoud

$-r_A = k C_A C_B^{1/2}$

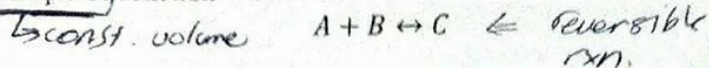
$-r_A = k \frac{C_{A0}(1-X)}{1-\frac{X}{3}} \left(\frac{\frac{C_{A0}}{2}(1-X)}{1-\frac{X}{3}} \right)^{1/2}$

$C_{A0} = \frac{y_{A0} P_0}{RT} = \frac{\frac{2}{3} \times 6 \text{ atm}}{0.08206 \times (260+273)}$
 $= 0.091 \text{ mol/dm}^3$

P3-16B

Calculate the equilibrium conversion and concentrations for each of the following reactions.

(a) The liquid-phase reaction

with $C_{A0} = C_{B0} = 2 \text{ mol/dm}^3$ and $K_C = 10 \text{ dm}^3/\text{mol}$.

$$C_{A0} = \frac{N_0}{V_0}$$

$$-r_A = K \left(C_A C_B - \frac{C_C}{K_C} \right) \stackrel{\text{at equilibrium}}{=} 0 \Rightarrow C_A^2 (1-x)^2 - \frac{C_{A0} x}{K_C} = 0$$

$$\Rightarrow C_A = C_{A0} (1-x)$$

$$(1-x)^2 - \frac{x}{2(10)} = 0$$

$$C_B = C_{A0} (\theta_B - x), \quad \theta_B = 1$$

$$\Rightarrow \boxed{x_e = 0.8}$$

$$\Rightarrow C_B = C_{A0} (1-x)$$

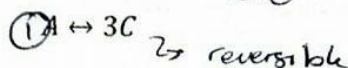
$$C_{Ae} = 2(1-0.8) = 0.4 \text{ mol/L} = C_{Be}$$

$$C_C = C_{A0} (\theta_C + x)$$

$$\Rightarrow C_C = C_{A0} x$$

$$C_{Ce} = 2(0.8) = 1.6 \text{ mol/L}$$

(b) The gas-phase reaction

 $\xrightarrow{\text{non-const. volume}}$ carried out in a flow reactor with no pressure drop. Pure A enters at a temperature of 400 K and 10 atm. At this temperature, $K_C = 0.25 (\text{dm}^3/\text{mol})^2$.

$$-r_A = k \left(C_A - \frac{C_C^3}{K_C} \right)$$

$$C_{A0} = \frac{y_{A0} P_0}{R T_0} = \frac{(1)(10 \text{ atm})}{0.08206 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}} \times 400 \text{ K}} = 0.305 \text{ mol/L}$$

$$C_A = \frac{C_{A0} (1-x)}{(1+\epsilon x)}$$

$$C_C = \frac{C_{A0} (\theta_C + 3x)}{(1+\epsilon x)}, \quad \theta_C = 0$$

Pure A enters

$$\boxed{F_{C0} = 0}$$

$$= \frac{3 C_{A0} x}{1+\epsilon x}$$

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

at equilibrium $-r_A = 0$

$$\frac{C_{A0} (1-x_e)}{1+2x_e} - \frac{(3 C_{A0} x_e)^3}{K_C (1+2x_e)^2} = 0 \Rightarrow x_e = 0.58$$

$$C_{Ae} = \frac{(0.305)(1-0.58)}{1+2(0.58)} = 0.06 \text{ mol/L}$$

(0905421) Chemical Reaction Engineering I - ICA # 11 (Chapter 3) - Dr. Linda Al-Hmoud

$$C_{Ce} = \frac{3(0.305)(0.58)}{1+2(0.58)} = 0.25 \text{ mol/L}$$

(0905421) Chemical Reaction Engineering I

In-Class Assessment # 13 (Chapter 4)

Partner (1) Name: CS M. Al-Jarrah Partner (2) Name: _____

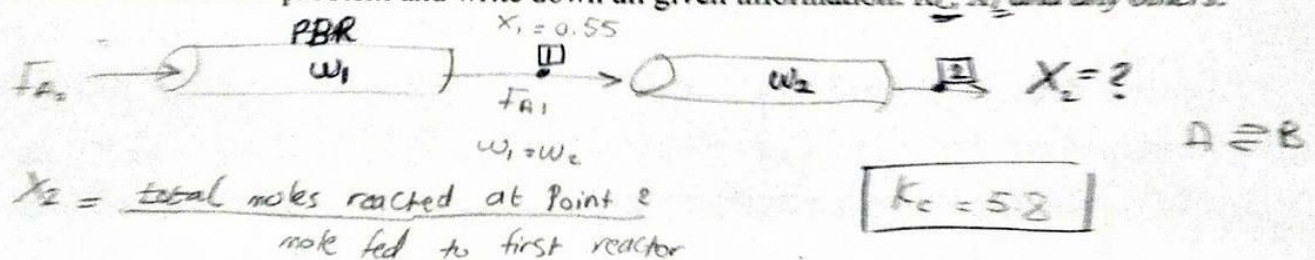
Identity (1) #: _____ Identity (2) #: _____

P4-13 Compound A undergoes a reversible isomerization reaction, $A \rightleftharpoons B$, over a supported metal catalyst. Under pertinent conditions, A and B are liquid, miscible, and of nearly identical density; the equilibrium constant for the reaction (in concentration units) is 5.8. In a fixed-bed isothermal flow reactor in which back mixing is negligible (i.e. plug flow), a feed of pure A undergoes a net conversion to B of 55%. The reaction is elementary. If a second, identical flow reactor at the same temperature is placed downstream from the first, what overall conversion of A would you expect if:

- (a) The reactors are directly connected in series? (Ans.: $X = 0.745$)
(b) The products from the first reactor are separated by appropriate processing and only the unconverted A is fed to the second reactor?

Solution (a): Follow the algorithm step-by-step:

0- Draw a sketch of the problem and write down all given information: K_C , X_1 , and any others.



$\Rightarrow X_2 = \frac{\text{total moles reacted at Point 2}}{\text{mole fed to first reactor}}$

1- Write the mole balance equation. Remember, the mole balance depends on the reactor type.

$$\frac{dx}{dw} = \frac{-r_A}{F_{A0}}$$

2- Write the rate law. Ask yourself: is it elementary or does it follow elementary rate law?

$$-r_A = k \left[C_A - \frac{C_B}{K_C} \right] \leftarrow \text{elementary}$$

3- Do the stoichiometry (i.e. write the concentration of species appearing in the rate law in terms of conversion). Ask yourself again: Is it liquid or gas phase? Constant volume or not?

Eq. V.V. $\hookrightarrow$ No δ

$$C_A = \frac{F_A}{V_0} = \frac{F_{A0}(1-x)}{V_0} = \underline{C_{A0}(1-x)}$$

$$C_B = \frac{F_B}{V_0} = \frac{F_{A0}x}{V_0} = \underline{C_{A0}x}$$

$$\therefore \theta_{A0} = \frac{F_{A0}}{F_{A0}} = 1 \quad \text{Product}$$

4. Now the last step: **COMBINE**. This means putting the concentrations in step (3) back in the rate law (2), and substituting this rate law, which is now in terms of conversion, in the mole balance you wrote in (1).

$$-r_A = K C_{A0} \left[1 - X - \frac{X}{K_c} \right]$$

$$\checkmark \frac{dx}{dw} = \frac{-r_A}{F_{A0}} = \frac{K C_{A0}}{F_{A0}} \left[1 - X \left(1 + \frac{1}{K_c} \right) \right]$$

$$\omega_1 \int_0^{x_1} dw = \int_0^{x_1} \dots$$

$$\omega_2 \int_{x_1}^{x_2} dw = \int_{x_1}^{x_2} \dots$$

5. Finally, solve the equation you got in (4) and find X_2 . $\Rightarrow \omega_1 = \omega_2$

$$\left\{ \omega_1 = \frac{F_{A0}}{K C_{A0}} \int_0^{x_1} \frac{dx}{\left[1 - \left(1 + \frac{1}{K_c} \right) x \right]} \right\} = \left\{ \omega_2 = \frac{F_{A0}}{K C_{A0}} \int_{x_1}^{x_2} \frac{dx}{\left[1 - \left(1 + \frac{1}{K_c} \right) x \right]} \right\}$$

$$\omega_1 = \frac{F_{A0}}{K C_{A0}} \frac{1}{\left(1 + \frac{1}{K_c} \right)} \ln \left(\frac{1}{1 - \left(1 + \frac{1}{K_c} \right) x_1} \right)$$

$$\div$$

$$\omega_2 = \frac{F_{A0}}{K C_{A0}} \frac{1}{\left(1 + \frac{1}{K_c} \right)} \ln \frac{\left(1 - \left(1 + \frac{1}{K_c} \right) x_1 \right)}{\left(1 - \left(1 + \frac{1}{K_c} \right) x_2 \right)}$$

cancel unknowns F_{A0} , K and C_{A0}

$$1 = \frac{\ln \left(\frac{1}{1 - 1.172 x_1} \right)}{\ln \left(\frac{1 - 1.172 x_1}{1 + 1.172 x_2} \right)}$$

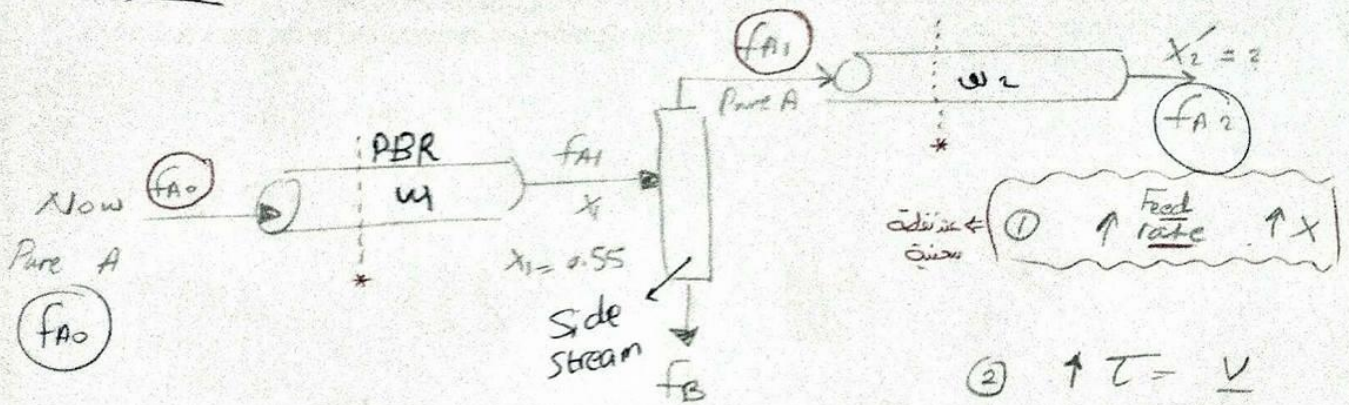
$$X_2 = \frac{\left[1 - \left(1 - \left(1 + \frac{1}{K_c} \right) x_1 \right)^2 \right]}{1 + \frac{1}{K_c}} \cdot \frac{\ln \left(\frac{1 - 1.172 x_1}{1 + 1.172 x_2} \right)}{\ln \left(\frac{1}{1 - 1.172 x_1} \right)}$$

Substitute $x_1 = 0.55$ and $K_c = 5.8$ $\cdot \frac{(1 - 1.172 x_1)^2}{1 - 1.172 x_1} = 1 + 1.172 x_2$

$$\boxed{X_2 = 0.745}$$

$$\boxed{\frac{1 - (1 - 1.172 x_1)^2}{1.172} = X_2}$$

Part 2



$$X_{\text{overall}} = \frac{f_{A0} - f_{A2}}{f_{A0}}$$

→ Conversion (X_2) based on f_{A1}

$$W_1 = \frac{f_{A0}}{K C_{A0}} \frac{1}{\left(1 + \frac{1}{K}\right)} \ln \left(\frac{1}{1 - \left(1 + \frac{1}{K}\right) X_1} \right)$$

$$W_2 = \frac{f_{A1}}{K C_{A0}} \int_0^{X_2} \frac{dx}{\left(1 - \left(1 + \frac{1}{K}\right) x\right)} = \frac{f_{A0}(1 - X_1)}{K C_{A0} \left(1 + \frac{1}{K}\right)} \ln \left(\frac{1}{1 - \left(1 + \frac{1}{K}\right) X_2} \right)$$

$$W_1 = W_2$$

$$f_{A1} = f_{A0}(1 - X_1)$$

$$1 = \frac{1}{(1 - X_1)} \frac{\ln \left(\frac{1}{1 - 1.172 X_1} \right)}{\ln \left(\frac{1}{1 - 1.172 X_2} \right)}$$

→ Substitute for f_{A1} and cancel f_{A0} , C_{A0} , K

One equation and one unknown Solving for X_2

$$X_2 = 0.768$$

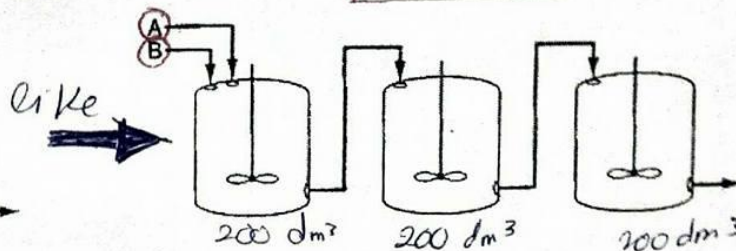
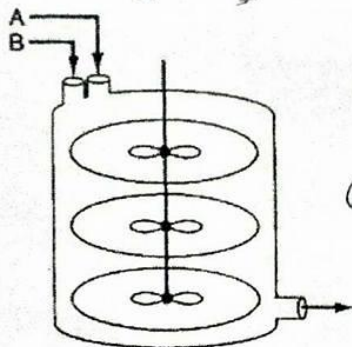
$$\Rightarrow X_{\text{overall}} = \frac{f_{A0} - f_{A2}}{f_{A0}} = \frac{f_{A0} - f_{A1}(1 - X_2)}{f_{A0}} = \frac{f_{A0} - f_{A0}(1 - X_1)(1 - X_2)}{f_{A0}} = 1 - (1 - X_1)(1 - X_2)$$

$$0.896 = 1 - (1 - 0.55)(1 - 0.77) = 1 - (1 - X_1)(1 - X_2)$$

Partner (1) Name: Osama Al-Hamoud Partner (2) Name: _____

Identity (1) #: _____ Identity (2) #: _____

The elementary (liquid-phase) reaction $A + B \rightarrow C$ is to be carried out in a CSTR with three impellers. The mixing patterns in the CSTR are such that it is modeled as three equal-sized CSTRs in series. Species A and B are fed in separate lines to the CSTR, which is initially filled with inert material. Each CSTR is 200 dm^3 and the volumetric flow to the first reactor is $10 \text{ dm}^3/\text{min}$ of A and $10 \text{ dm}^3/\text{min}$ of B.



$$-r_A = k C_A C_B = k C_{A0} (1-x) (C_{A0} (1-x))$$

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

A. What is the conversion of A?

B. If the three tanks were connected in parallel with A and B split equally among the three reactors, what will be the conversion of A?

Additional Information

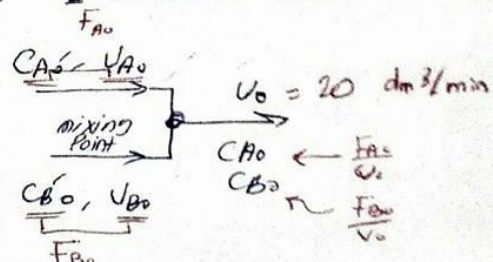
$$C_{A0} = C_{B0} = 2.0 \text{ mol/dm}^3$$

$$k = 0.025 \text{ dm}^3/\text{mol/min}$$

$$V_{A0} = 10, V_{B0} = 10$$

$$V_0 = 10 + 10 = 20 \text{ dm}^3/\text{min}$$

$$V_0 = V_{A0} + V_{B0} = 20 \text{ dm}^3/\text{min}$$



$$C_{A0} = \frac{F_{A0}}{V_0} = \frac{(C_{A0})(V_{A0})}{V_0}$$

$$C_{A0} = \frac{F_{A0}}{V_0} = \frac{2 \times 10}{20} \text{ mol/dm}^3 = 1 \text{ mol/dm}^3 = C_{B0}$$

conversion for (1) reactors in series:

$$X = 1 - \frac{1}{(1 + Da)^n}$$

2nd order respect to A

$$Da = k C_{A0} \tau = 0.025 \frac{\text{dm}^3}{\text{mol min}} \times \frac{1 \text{ mol}}{\text{dm}^3} \times \frac{200}{20} \text{ min} = 0.25$$

$$Da = 0.25$$

$$= 1 - \left(\frac{1}{(1 + 0.25)^3} \right) = 0.488 = X$$

only if they have same volume.

$$(b) \quad V_{\text{total}} = \frac{F A_0 X}{k C A_0^2 (1-X)^2} =$$

$$\begin{matrix} \text{total} \\ 200 \times 3 \end{matrix} \rightarrow 600 = \frac{20 X}{0.025 (1) (1-X)^2} \quad \equiv \quad 200 = \frac{(20/3) X}{(0.025) (1) (1-X)^2}$$

$$\boxed{X = 0.333}$$

Parallel

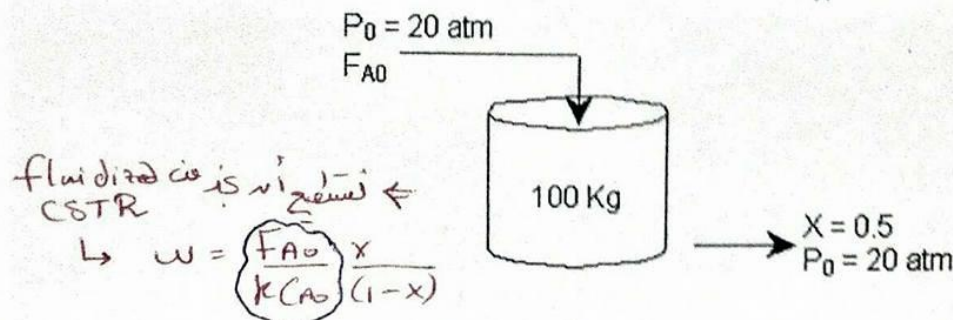
(0905421) Chemical Reaction Engineering I

In-Class Assessment # 16 (Chapter 4)

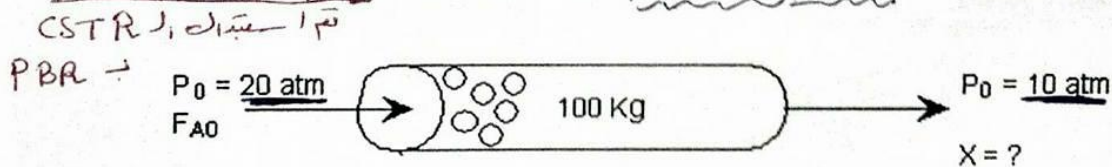
Partner (1) Name: Sayid Ali Partner (2) Name: Eyad

Partner (1) ID #: Partner (2) ID #:

The elementary isomerization reaction $A \rightarrow B$ is carried out isothermally at 20 atm in a fluidized CSTR containing 100 kg of catalyst, where 50% conversion is achieved.



It is proposed to replace the CSTR with a packed bed reactor



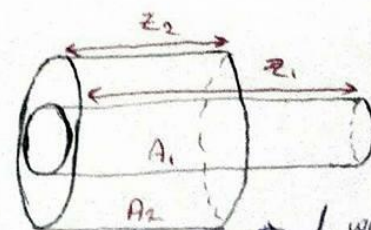
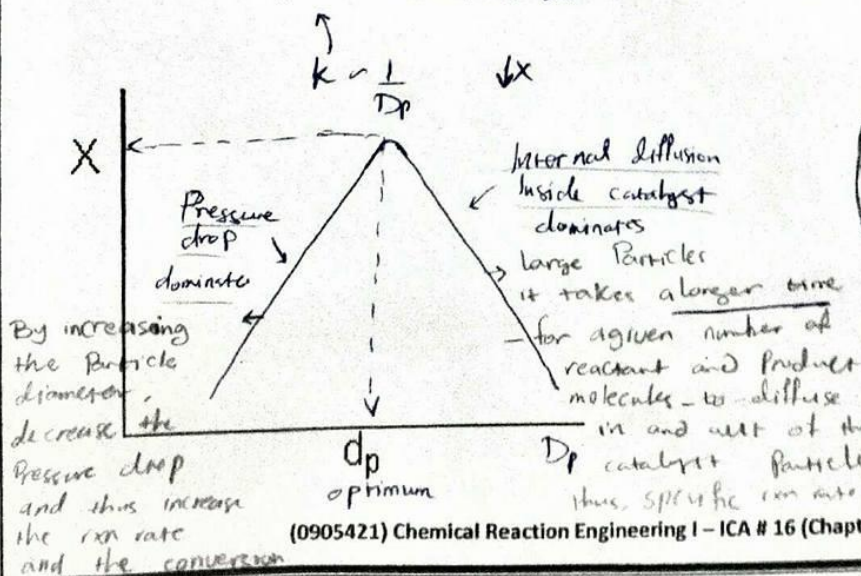
The entering pressure was 20 atm and the exit pressure was found to be 10 atm.

A. What would be the conversion in the PBR if there were NO pressure drop?
Hint 1: What information can you obtain from the CSTR?

B. What will be the conversion in the new PBR with pressure drop?
Hint 2: How do you calculate the pressure drop parameter, α ?

C. Plot the conversion as a function of particle diameter assume everything else is unchanged. Why does the $X-d_p$ curve look the way it does?
mass transfer (rate law)

D. Suppose you could choose another pipe diameter to hold the same amount of catalyst. Would you choose a larger or smaller pipe diameter, or would you use the current pipe diameter? Explain.



$$A_1 < A_2$$

$$D_1 < D_2$$

$$W_1 = W_2$$

I will choose the larger diameter because the pressure drop increase as diameter increase and decrease conversion

classwork (16)



$W = 100$ kg of catalyst

$P = 10$ atm

fluidized CSTR $\Rightarrow W = \frac{F_{A0} X}{-r_A}$

① mole balance :

$$F_{A0} \frac{dx}{dw} = -r_A$$

② rate law :

$$-r_A = k C_A$$

③ stoichiometry :

$$C_A = C_{A0} \frac{(1-X)}{(1+\epsilon X)} \quad \text{y} \quad \frac{T_0}{T_1} \quad ; \quad \epsilon = (1-1) y_{A0}$$

NO ΔP Isothermal $\epsilon = \text{zero}$

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

④ combine

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

$$F_{A0} \frac{dx}{dw} = \frac{k C_{A0}}{1} (1-X)$$

$\Rightarrow$ From fluidized bed:

$$W = \frac{F_{A0} X}{-r_A}$$

$$100 = \frac{F_{A0} (0.5)}{k C_{A0} (1-X)} \quad \Rightarrow \quad 100 = \frac{F_{A0}}{k C_{A0}} \frac{0.5}{(1-0.5)} \quad \Rightarrow \quad \frac{F_{A0}}{k C_{A0}} = 100$$

$$\int_0^X \frac{dx}{(1-x)} = \frac{k C_{A0}}{F_{A0}} \int_0^W dw$$

$$-\ln(1-x) \Big|_0^X = \frac{1}{100} W$$

$$-\ln(1-x) = \frac{100}{100}$$

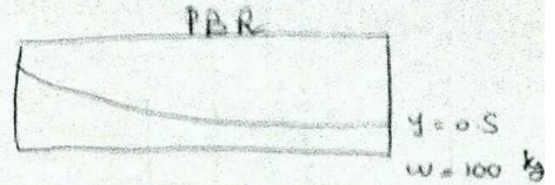
$$-\ln(1-x) = 1$$

$$\boxed{X = 0.632}$$

(B) with Pressure drop (y)

$$y = 1$$

$$w = 0$$



① mole balance: $F_{A0} \frac{dx}{dw} = -r'_A$

② rate law: $-r'_A = k C_A$

③ stoichiometry: $C_A = C_{A0} \frac{(1-x)}{(1+\epsilon x)}$ $\frac{T}{T_0}$ $\epsilon = 2.0$
 Isothermal

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

④ combine: $-r'_A = k C_{A0} (1-x)$

$$F_{A0} \frac{dx}{dw} = k C_{A0} (1-x) y \quad ; \quad y = \sqrt{1-\alpha w}$$

$$\int_0^x \frac{dx}{1-x} = \frac{k C_{A0}}{F_{A0}} \int_0^w y dw$$

$$-\ln(1-x) \Big|_0^x = \frac{1}{100} \int_0^w y dw$$

$$-\ln(1-x) = \frac{1}{100} \int_0^w \frac{dw (1-\alpha w)^{1/2}}{(1-\alpha w)^{1/2}}$$

$$w = \frac{F_{A0} x}{-r'_A} = \frac{F_{A0} x}{k C_{A0} (1-x)}$$

$$100 = \frac{F_{A0} \cdot 0.5}{k C_{A0} (1-0.5)}$$

$$100 = \frac{F_{A0}}{k C_{A0}}$$

$$\frac{F_{A0}}{k C_{A0}} = 100$$

$$-\ln(1-x) = \frac{1}{100} \frac{1}{(0.5)(-\alpha)} \int_0^w (1-\alpha w)^{1/2} dw$$

$$-\ln(1-x) = \frac{1}{(50)(-\alpha)} \left((1-\alpha w)^{1/2} - 1 \right)$$

$$; \alpha = ?$$

$$y = \sqrt{1-\alpha w}$$

$$\frac{16}{20} = \sqrt{1-\alpha(100)}$$

$$\boxed{\alpha = 7.5 \times 10^{-3} \text{ kg}^{-1}}$$

on calculator

$$-\ln(1-x) = \frac{1}{100} (50)$$

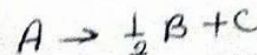
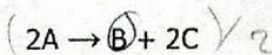
$$\Rightarrow \boxed{X = 0.393}$$

Partner (1) Name: Osama Partner (2) Name: _____

Partner (1) ID #: _____ Partner (2) ID #: _____

What four things are wrong with this membrane reactor solution?

The gas phase elementary reaction



$$\epsilon = \frac{1}{2} + \nu - \left(\frac{1}{2} \right) \left(\frac{1}{2} \right) = \frac{1}{4}$$

$$\boxed{\epsilon \neq 0}$$

$$\boxed{\epsilon = 0.25}$$

$$\Rightarrow C_{t0} = 0.4 \frac{\text{mol}}{\text{dm}^3}$$

$$\Rightarrow F_{A0} = \frac{10 \text{ mol}}{\text{s}}$$



sweep gas (inert gas)

take (B) $\Rightarrow C_{B0} = 0$

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 $(k_c = 1.5 \text{ dm}^3/\text{kg} \cdot \text{s})$

Proposed Solution $\Rightarrow$ Differential equations

$$1 \quad d(F_A)/d(W) = r_A \quad \checkmark$$

$$2 \quad d(F_B)/d(W) = r_B - R_B \quad \checkmark$$

$$3 \quad d(F_C)/d(W) = r_C \quad \checkmark$$

 $\Rightarrow$ Explicit equations

$$F_I \quad \times \quad 1 \quad F_t = F_A + F_B + F_C + F_I$$

$$2 \quad k_A = 2.5 \quad \checkmark$$

$$3 \quad C_{t0} = 0.4 \quad \checkmark$$

$$4 \quad \alpha = 0.019 \quad \checkmark$$

$$5 \quad y = (1 - \alpha W)^{0.5} \quad \checkmark$$

$$6 \quad C_B = C_{t0} F_B y / F_t \quad \checkmark$$

$$7 \quad C_A = C_{t0} F_A y / F_t \quad \checkmark$$

$$8 \quad r_B = k_A C_A \quad \checkmark$$

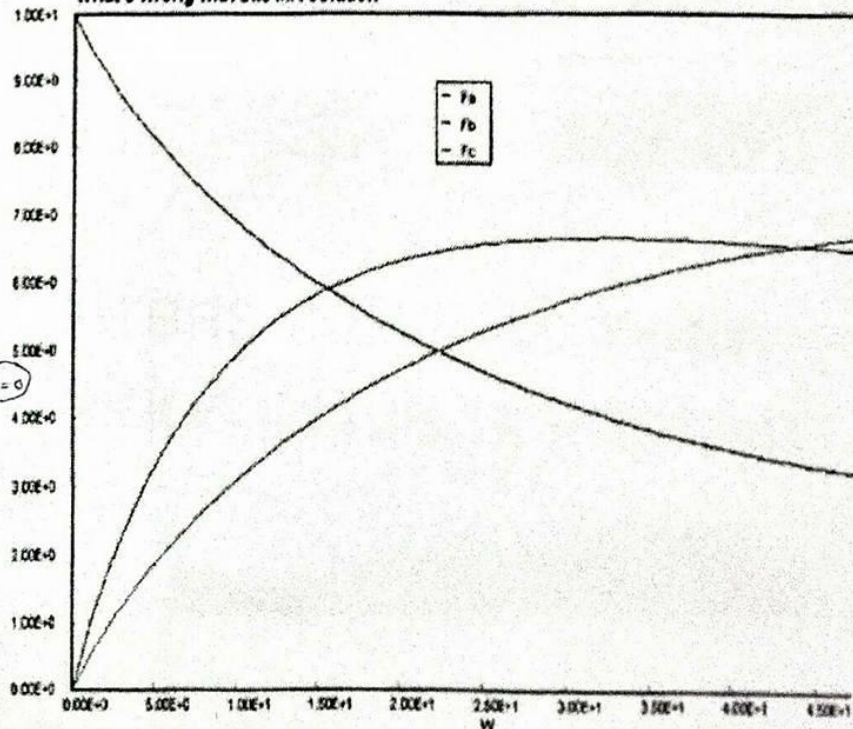
$$9 \quad r_A = -r_B/2 \quad \checkmark$$

$$10 \quad r_C = -r_A \quad \checkmark$$

$$11 \quad k_c = 1.5 \quad \checkmark$$

$$12 \quad R_B = k_c C_B \quad \checkmark$$

What's wrong with this MR solution



① mole balance

$$\frac{dF_A}{dw} = -r_A$$

$$\frac{dF_B}{dw} = r_B - R_B$$

$$\frac{dF_C}{dw} = r_C$$

② rate law

$$-r_A = k C_A^2$$

$$r_A = -k C_A^2$$

$$R_B = k_c C_B$$

relative rate

$$\frac{r_A}{-2} = \frac{r_B}{1} = \frac{r_C}{2}$$

$$r_B = \frac{r_A}{-2} = \frac{r_C}{2}$$

$$R_B = k_c C_B$$

③ Stoich.

$$C_A = C_{T0} \frac{F_A}{F_T} y$$

$$C_B = C_{T0} \frac{F_B}{F_T} \delta$$

$$F_T = F_A + F_B + F_C + F_I$$

$$E = y_A \delta$$

$$= \left(\frac{1}{2}\right) \left(\frac{1}{2}\right)$$

$$E = 0.25 \neq \text{zero}$$

$$\frac{dy}{dw} = \frac{-y}{2y} \frac{F_T}{F_{T0}}$$

→ evaluated parameters

$$F_{A0} = 10 \text{ mol/s}$$

$$F_{B0} = 0$$

$$F_{C0} = 0$$

$$w(0) = 0$$

$$w(t) = 50 \text{ kg}$$

$$y(0) = 1$$

$$k = 2.5 \frac{\text{dm}^3}{\text{mol} \cdot \text{kg} \cdot \text{s}}$$

$$k_c = 1.5 \frac{\text{dm}^3}{\text{kg} \cdot \text{s}}$$

$$d = 0.019 \text{ kg}^{-1}$$

$$C_{T0} = 0.4 \text{ mol/dm}^3$$

$$F_{T0} = 10 \text{ mol/s}$$

(0905421) Chemical Reaction Engineering I

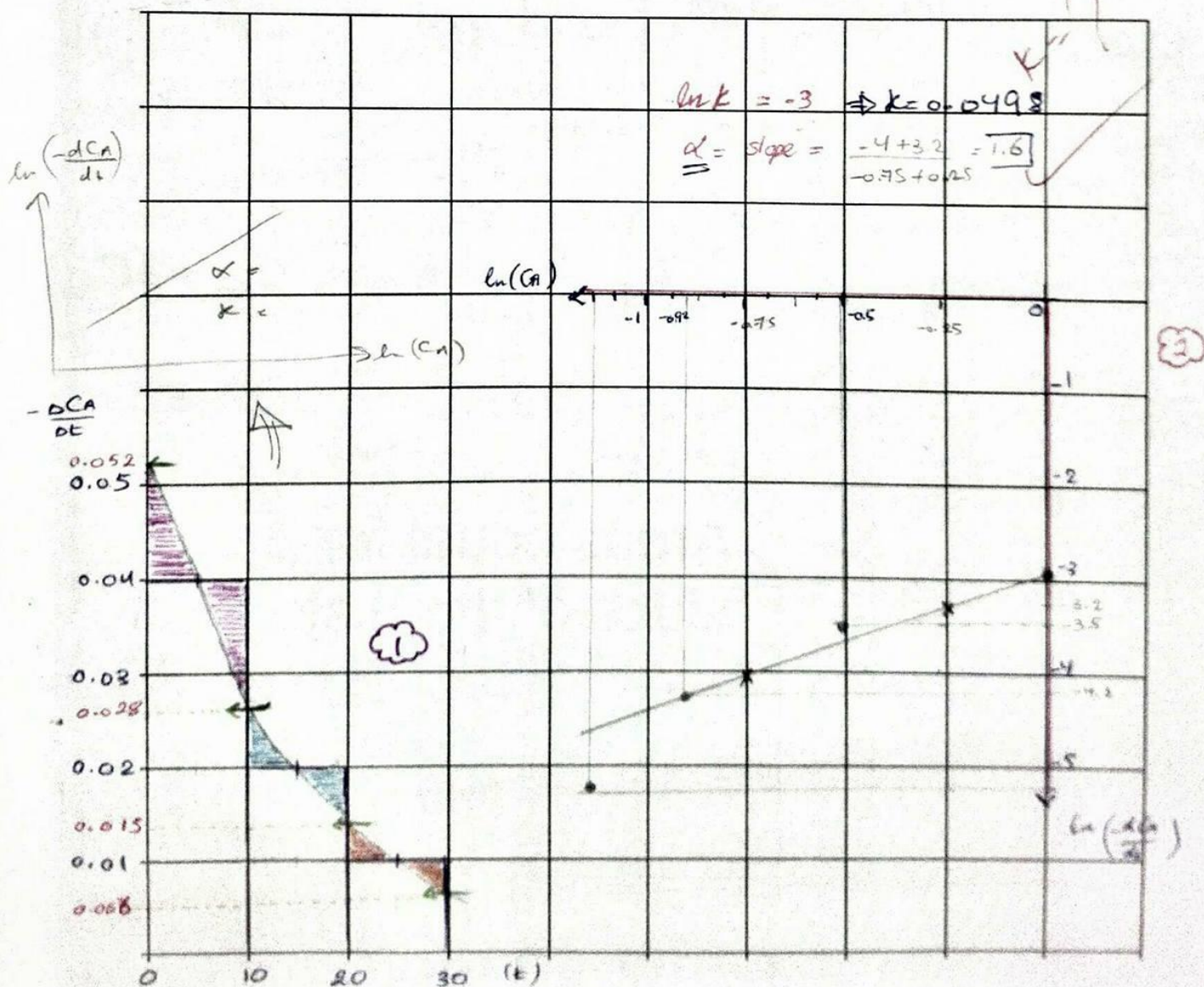
In-Class Assessment # 18 (Chapter 5)

Partner (1) Name: سعدية Partner (2) Name: _____

Partner (1) ID #: 0153646 Partner (2) ID #: _____

The reaction $A \rightarrow B$ is carried out in a constant volume batch reactor. Determine the reaction order and specific reaction rate from the following data.

t (min)	0	10	20	30	t (min)	0	10	20	30
C_A (mol/dm ³)	1	0.6	0.4	0.3	$\ln(C_A)$	0	-0.51	-0.92	-1.2
$-\Delta C_A / \Delta t$		0.04	0.02	0.01	$-dC_A/dt$	0.05	0.03	0.015	0.008
$-dC_A/dt$	0.052	0.028	0.015	0.008	$\ln(-dC_A/dt)$	-2.99	-3.5	-4.2	-5.3
$\ln(-dC_A/dt)$									



2. Numerical differentiation formulas

Time (min)	t_0	t_1	t_2	t_3	t_4	t_5
Concentration (mol/dm ³)	C_{A0}	C_{A1}	C_{A2}	C_{A3}	C_{A4}	C_{A5}

The three-point differentiation formulas¹

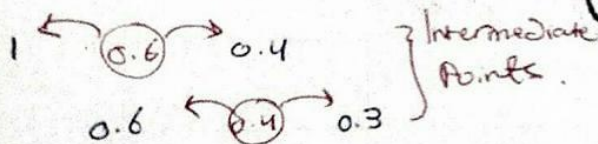
Initial point:



$$\left(\frac{dC_A}{dt}\right)_{t_0} = \frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t}$$

$$\left(\frac{dC_A}{dt}\right)_{i=1} = \frac{-3(1) + 4(0.6) - 0.4}{2(10)} = -0.05$$

Interior points:



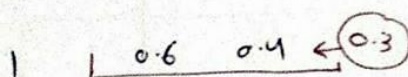
$$\left(\frac{dC_A}{dt}\right)_{t_{i-2}} = \frac{1}{2\Delta t} [(C_{A(i+1)} - C_{A(i-1)})]$$

$(2+1)=3$ third point $(2-1)=1$ first point
 2nd point

$$\left(\frac{dC_A}{dt}\right)_{i=2} = \frac{0.4 - 1}{2(10)} = -0.03$$

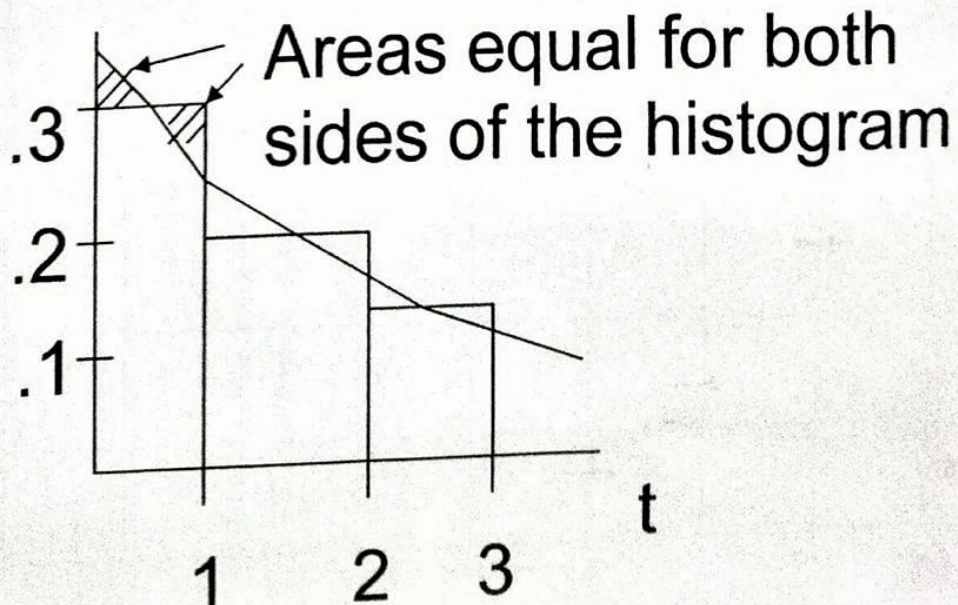
$$\left(\frac{dC_A}{dt}\right)_{i=3} = \frac{0.3 - 0.6}{2(10)} = -0.015$$

Last point:



$$\left(\frac{dC_A}{dt}\right)_{i=4} = \frac{6(0.6) - 4(0.4) + 3(0.3)}{2(10)} = -0.005$$

$$-\frac{\Delta C_A}{\Delta t}$$



(0905421) Chemical Reaction Engineering I

In-Class Assessment # 19 (Chapter 5)

Partner (1) Name: Osama Al-Jarrah Partner (2) Name: _____

Partner (1) ID #: 0153646 Partner (2) ID #: _____

P5-7 The liquid-phase reaction of methanol and triphenyl takes place in a batch reactor at 25°C



For an equal molar feed, the following concentration-time data was obtained for methanol:

$C_A = C_B - (1 - \nu)$
(B) →

t (h)	0	0.278	1.389	2.78	8.33	16.66
C _A (mol/dm ³)	0.1	0.95	0.816	0.707	0.50	0.37

$$\begin{aligned} -r_A &= k C_A^\alpha C_B^\beta \\ &= k C_A^\alpha C_A^\beta \\ &= k C_A^{(\alpha+\beta)} \end{aligned}$$

The following concentration-time data was carried out for an initial methanol concentration of 0.01 mol/dm³, and an initial triphenyl of 0.1 mol/dm³:

$C_{A0} = 0.01 \text{ mol/L}$
 $C_{B0} = 0.1 \text{ mol/L}$
 $C_B = C_{B0} = \text{constant}$

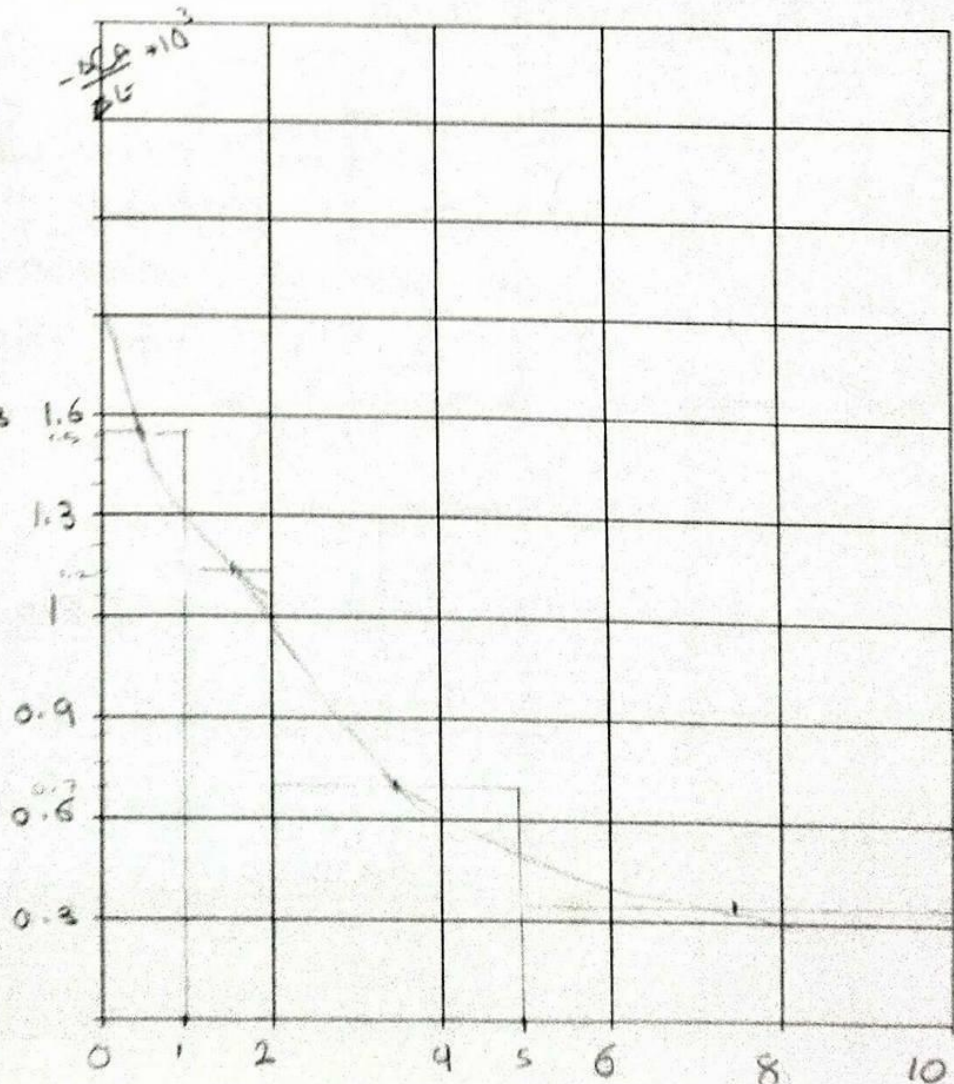
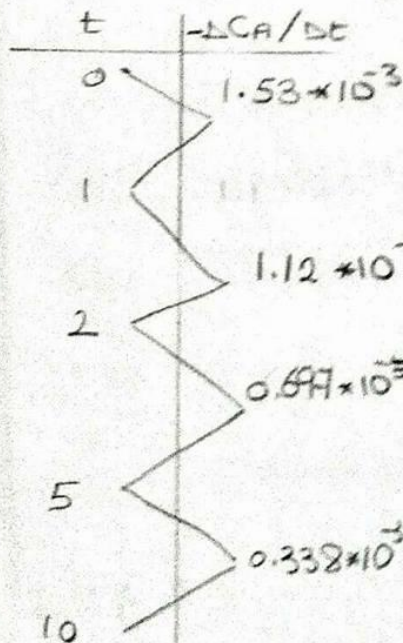
t (h)	0	1	2	5	10
C _A (mol/dm ³)	0.01	0.00847	0.00735	0.00526	0.00357

دالة التفاعل
الدرجة

Determine the rate law and rate law parameters.

$$-r_A = k' C_A^\alpha$$

Graphical



P5-10 The gas-phase decomposition $A \rightarrow B + 2C$ is carried out in a constant volume batch reactor. Runs 1 through 5 were carried out at 100°C , while run 6 was carried out at 110°C .

(a) From the data in the table, determine the reaction order and specific reaction rate.

(b) What is the activation energy for this reaction? α k

at 100°C

also k at 110°C
(different temp. at 110°C)

Run	Initial Concentration, C_{A0} (mol/L)	Half-Life, $t_{1/2}$ (min)	$\ln C_{A0}$	$\ln t_{1/2}$
1	0.0250	4.1	-3.68	1.41
2	0.0133	7.7	-4.3	2.04
3	0.010	9.8	-4.6	2.28
4	0.05	1.96	-2.99	0.67
5	0.075	1.3	-2.6	0.26
6	0.025	2.0	-3.68	0.693

$$\Rightarrow \text{slope} = \frac{1.7 - 1}{-4.1 + (3.4)} = -1$$

[9]

$\Rightarrow$ 2nd order

$$\Rightarrow \text{slope} = 1 - \alpha$$

$$-1 = 1 - \alpha$$

$\alpha = 2$ order of rxn. (2nd order)

$$\ln t_{1/2} = \ln \frac{2^{\alpha-1} - 1}{k(\alpha-1)} + (1-\alpha) \ln C_{A0}$$

$$(0.693) = \ln \frac{2^2 - 1}{k(1)} + (-1)(-3.68)$$

$$k_2 = 19.83 \text{ dm}^3/\text{mol} \cdot \text{min}$$

[b] From Arrhenius eq:

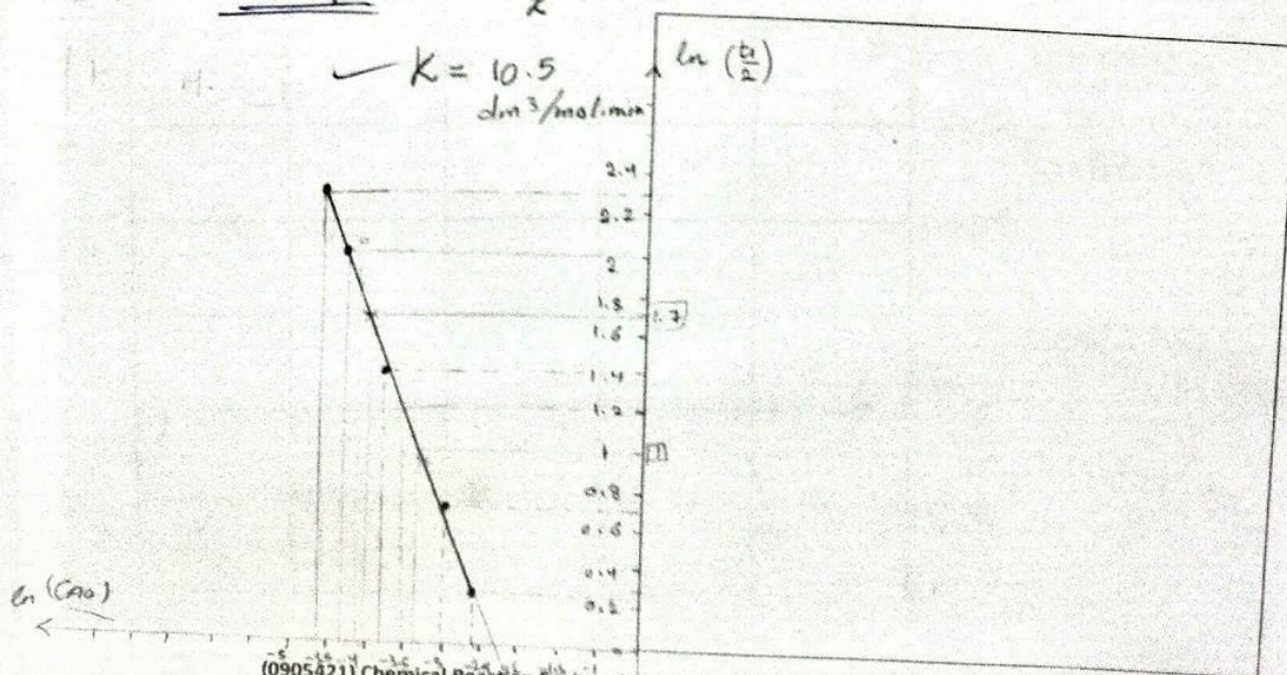
$$\ln \left(\frac{k_1}{k_2} \right) = -\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

$$\ln \left(\frac{10.5}{19.83} \right) = \frac{-E}{8.314} \left(\frac{1}{373} - \frac{1}{383} \right)$$

$$E = 75518.3 \text{ J/mol}$$

from Intercept $\Rightarrow \ln \frac{2^2 - 1}{k} =$

$$K = 10.5 \text{ dm}^3/\text{mol} \cdot \text{min}$$



The University of Jordan
School of Engineering
Chemical Engineering Department

(0905421) Chemical Reaction Engineering I

In-Class Assessment # 21 (Chapter 6)

Partner (1) Name: Baqir Partner (2) Name: _____

Partner(1) ID #: _____ Partner(2) ID #: _____

P6-12 The following liquid-phase reactions were carried out in a CSTR at 325 K.



$$-r_{1A} = k_{1A} C_A$$

$$k_{1A} = 7.0 \text{ min}^{-1}$$



$$r_{2D} = k_{2D} C_A C_C^2$$

$$k_{2D} = 3.0 \text{ L}^2/(\text{mol}^2 \cdot \text{min})$$



$$r_{3E} = k_{3E} C_D C_C$$

$$k_{3E} = 2.0 \text{ L}/(\text{mol} \cdot \text{min})$$

The concentrations measured inside the reactor were $C_A = 0.10$, $C_B = 0.93$, $C_C = 0.51$, and $C_D = 0.049$ all in mol/L.

(a) What are r_{1A} , r_{2A} , and r_{3A} ?

$$r_{1A} = -k_{1A} C_A$$

$$r_{3A} = 0$$

$$\frac{r_{2A}}{-1} = \frac{r_{2D}}{3}$$

$$r_{2A} = -\frac{k_{2D}}{3} C_A C_C^2$$

(b) What are r_{1B} , r_{2B} , and r_{3B} ?

$$r_{1B} = \frac{k_{1A}}{3} C_A$$

→ be careful for the signs

$$r_{2B} = 0$$

$$r_{3B} = 0$$

(c) What are r_{1C} , r_{2C} , and r_{3C} ?

$$r_{1C} = \frac{k_{1A}}{3} C_A$$

$$r_{2C} = -\frac{2}{3} k_{2D} C_A C_C^2$$

$$r_{3C} = -k_{3E} C_D C_C$$

(d) What are r_{1D} , r_{2D} , and r_{3D} ?

$$r_{1D} = 0$$

$$r_{2D} = k_{2D} C_A C_C^2$$

$$r_{3D} = \frac{4}{3} k_{3E} C_D C_C$$

(e) What are r_{1E} , r_{2E} , and r_{3E} ?

$$r_{1E} = 0$$

$$r_{2E} = 0$$

$$r_{3E} = k_3 C_D C_C$$

(f) What are the net rates of formation of A, B, C, D, and E?

$$r_{A, \text{net}} = -k_1 C_A - \frac{k_2}{3} C_A C_C^2$$

$$r_{B, \text{net}} = \frac{k_1}{3} C_A$$

$$r_{C, \text{net}} = \frac{k_1}{3} C_A - \frac{2}{3} k_2 C_A C_C^2 - k_3 C_D C_C$$

$$r_{D, \text{net}} = k_2 C_A C_C^2 - \frac{4}{3} k_3 C_D C_C$$

$$r_{E, \text{net}} = k_3 C_D C_C$$

(g) The entering volumetric flow rate is 100 L/min and, the entering concentration of A is 3 M . What is the CSTR reactor volume?

Parts (h), (i), (j) are HOMEWORK! (Solve them using POLYMATH or MATLAB)

$$v_0 = 100 \text{ L/min}$$

$$C_{A0} = 3 \text{ mol/L}$$

$$V_{\text{CSTR}} = ?$$

$$C_C = 0.51 \text{ mol/L}$$

$$C_A = 0.1 \text{ mol/L}$$

$$V = \frac{F_{A0} - F_A}{-r_{A, \text{net}}} = \frac{(C_{A0} - C_A) v_0}{-r_A} = \frac{F_{C0} - F_{C\infty}}{r_{A, \text{net}}}$$

$$= \frac{(3 - 0.1) 100}{k_1 C_A + \frac{k_2}{3} C_A C_C^2}$$

$$= 460 \text{ L}$$

$$= \frac{(3 - 0.1) 100}{(7)(0.1) + \frac{3}{3} (0.1) (0.51)^2}$$

$$V_{\text{CSTR}} = 399.4 \text{ L}$$

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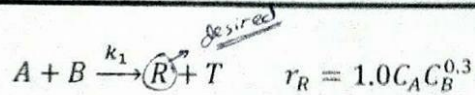
(0905421) Chemical Reaction Engineering I

In-Class Assessment # 21 (Chapter 6)

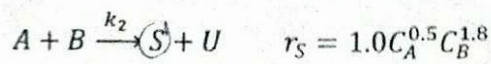
Partner (1) Name: Samir Partner (2) Name: _____

Identity (1) #: _____ Identity (2) #: _____

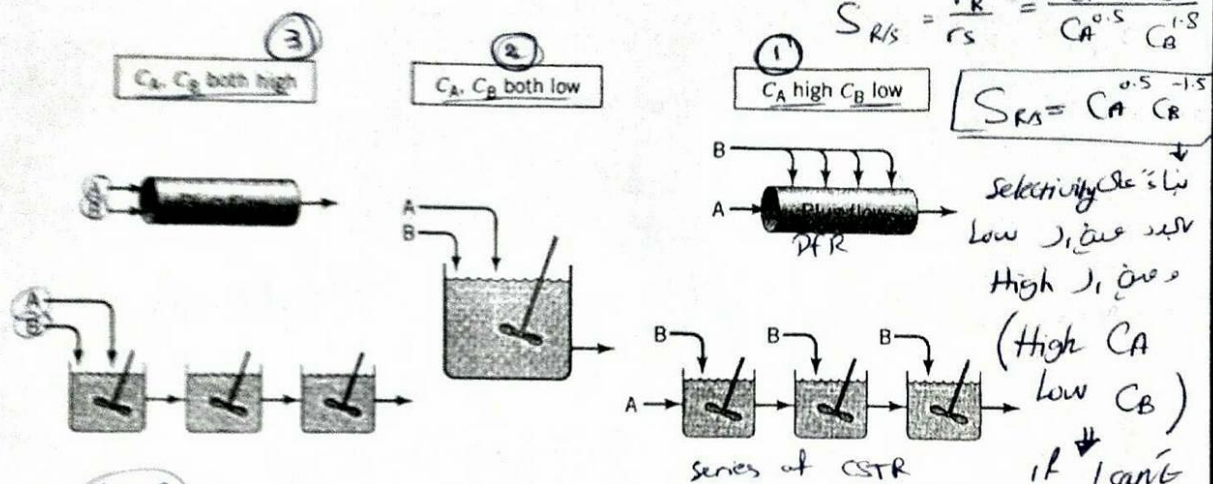
The desired liquid-phase reaction



is accompanied by the unwanted side reaction



- a. From the standpoint of favorable product distribution, order the contacting schemes shown below from the most to the least desirable.



- b. For 90% conversion of pure A and pure B, both of which is fed from a stream of 20 mol/L concentration, what will be the overall yield of R, C_R , and C_S in a plug flow reactor, PFR.

$$\begin{aligned} C_{A0} &= 20 \text{ mol/L} \\ C_{B0} &= 20 \text{ mol/L} \\ C_{A0} &= 10 \text{ mol/L} \\ C_{B0} &= 10 \text{ mol/L} \end{aligned} \quad X_A = 90\% \Rightarrow C_A = 1 \text{ mol/L} = C_B$$

1. PFR $Y_R = \frac{F_R}{F_{A0} - F_A} = \frac{C_R}{C_{A0} - C_A}$

$$\frac{dV}{r_A} = \frac{dF_A}{-r_A} = \frac{20 dC_A}{-C_A^{1.5} - C_A^{2.3}} \quad ; C_A = C_B$$

(low C_A)
(low C_B)
because the effect for $C_B^{-1.5}$ larger than $C_A^{0.5}$.

class work # (21)

(b)

$$\begin{aligned} \longrightarrow C_{A0} &= 20 \text{ mol/L} \\ \longrightarrow C_{B0} &= 20 \text{ mol/L} \end{aligned} \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \begin{array}{l} C_{A0} = 10 \text{ mol/L} \\ C_{B0} = 10 \text{ mol/L} \end{array}$$

$$X_A = 0.9$$

assume same volume flow rate v_0

$$\begin{aligned} C_A &= C_{A0}(1-X) \\ &= 10(1-0.9) \end{aligned}$$

$$\boxed{C_A = 1 \text{ mol/L}} = \underline{C_B}$$

(1) PFR: (Plug flow reactor)

overall yield of R:

$$Y_R = \frac{F_R}{F_{A0} - F_A} = \frac{v_0 C_R}{v_0 C_{A0} - v_0 C_A} = \frac{\boxed{C_R}^{?}}{\underset{10}{C_{A0}} - \underset{1}{C_A}} = \frac{\cancel{1.7}}{10-1} = \frac{0.19}{\text{very Low}} = \underline{19\%}$$

⇒ (1) mole balance

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

$$dV = \frac{dF_A}{r_A} = \frac{v_0 dC_A}{-C_A^{0.3} C_B^{0.5} - C_A^{1.3} C_B^{2.3}} = \frac{v_0 dC_A}{-C_A^{1.3} - C_A^{2.3}}$$

$\boxed{C_A = C_B}$

$$\boxed{dV = \frac{dF_A}{r_A} = \frac{dF_R}{r_R} = \frac{dF_S}{r_S}} +$$

I need to know C_R :

$$\begin{aligned} \frac{dF_A}{r_A} &= \frac{dF_R}{r_R} \Rightarrow \frac{v_0 dC_A}{-(C_A^{1.3} + C_A^{2.3})} = \frac{v_0 dC_R}{C_A^{1.3}} \Rightarrow \frac{-dC_A}{C_A^{1.3}(1+C_A)} = \frac{dC_R}{C_A^{1.3}} \\ \int_{C_{A0}}^{C_A} \frac{-dC_A}{1+C_A} &= \int_{C_{A0}}^{C_R} dC_R \\ \Rightarrow \int_{C_{A0}=10}^{C_A=1} \frac{dC_A}{1+C_A} &= C_R \end{aligned}$$

$$\ln\left(\frac{1+C_{A0}}{1+C_A}\right) = C_R \Rightarrow C_R = \ln\left(\frac{1+10}{1+1}\right)$$

$$\boxed{C_R = 1.7 \text{ mol/L}}$$

⇒ because the stich. are equivalent

$$C_{A0} = C_A + C_R + C_S$$

$$10 = 1 + 7.1 + C_S$$

$$C_S = 7.3 \text{ mol/L}$$

② mixed reactor (CSTR):

① mole balance

$$V = \frac{F_{A0} - F_A}{-r_A} = \frac{F_R - F_{A0}}{r_R}$$

$$\frac{20(C_{A0} - C_A)}{C_A^{1.3} + C_A^{2.3}} = \frac{20C_R}{C_A^{1.3}} \Rightarrow C_R = \frac{C_{A0} - C_A}{(1 + C_A)} = \frac{10 - 1}{1 + 1} =$$

$$C_R = 4.5 \text{ mol/L}$$

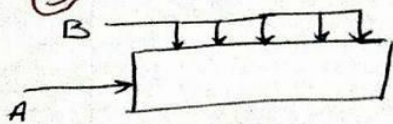
$$C_{A0} = C_A + C_R + C_S$$

$$10 = 1 + 4.5 + C_S$$

$$C_S = 4.5 \text{ mol/L}$$

⇒ Yield of R ⇒ $\underline{Y_R} = \frac{F_R}{F_{A0} - F_A} = \frac{C_R}{C_{A0} - C_A} = \frac{4.5}{10 - 1} = \underline{0.5}$ 50%

③



$$C_{A0} = ?$$

$$\text{as base} = 1 \text{ L/min}$$

$$C_B = 1 \text{ mol/L}$$

$$C_A = 1 \text{ mol/L}$$

$$C_A \neq C_B$$

$$r_R = C_A^{0.3} = C_A$$

$$-r_A = r_R + r_S$$

$$-r_A = C_A + C_A^{0.5}$$

total molar flow rate

$$C_{A0} = \frac{v_0 C_{A0}}{v_{\text{total}}} = \frac{(1)(20)}{1 + 0.05} = 19 \frac{\text{mol}}{\text{L}}$$

$C_{A0} = 19 \text{ mol/L}$
 $v_0 = 1 \text{ L/min}$
 $C_{B0} = 1 \text{ mol/L}$
 $v_0 = 0.05 \text{ L/min}$
 1 stream
 20 streams

$$\frac{dC_A}{r_A} = \frac{dC_R}{r_R} \Rightarrow \int_{C_{A0}}^{C_A} \frac{-dC_A}{C_A + C_A^{0.5}} = \int_0^{C_R} \frac{dC_R}{C_A}$$

$$\int_{C_{A0}}^{C_A} \frac{dC_A}{1 + C_A^{-0.5}} = C_R \Rightarrow \text{on calculator}$$

$$C_R = 13.25 \text{ mol/L}$$

$$Y_R = \frac{13.25}{19 - 1} = 0.74$$

$$C_S = C_{A0} - C_A - C_R = 19 - 1 - 13.25 = 4.75 \text{ mol/L}$$

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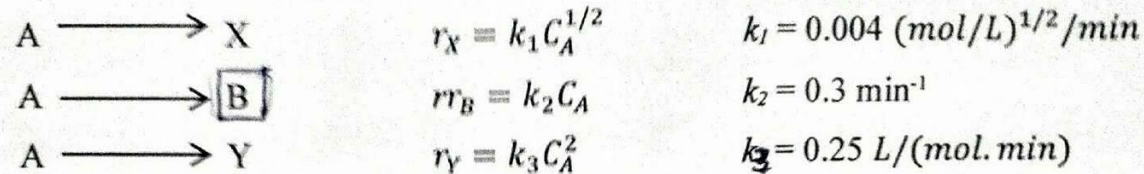
(0905421) Chemical Reaction Engineering I

In-Class Assessment # 20 (Chapter 6)

Partner (1) Name: Samir, 27 July Partner (2) Name: _____

Partner (1) ID #: _____ Partner (2) ID #: _____

P6-6 Consider the following system of gas-phase reactions:



B is the desired product, and X and Y are foul pollutants that are expensive to get rid of. The given specific reaction rates are at 27 °C. The reaction system is to be operated at 27 °C and 4 atm. Pure A enters the system at a volumetric flow rate of 10 L/min.

- Sketch the instantaneous selectivities ($S_{B/X}$, $S_{B/Y}$, and $S_{B/XY} = r_B / (r_X + r_Y)$) as a function of the concentration of A, C_A .
- Consider a series of reactors. What should be the volume of the first reactor?
- What are the effluent concentrations of A, B, X, and Y from the first reactor?
- What is the conversion of A in the first reactor?
- If 99% conversion of A is desired, what reaction scheme and reactor sizes should you use to maximize $S_{B/XY}$?
- Suppose that $E_1 = 20,000 \text{ cal/mol}$, $E_2 = 10,000 \text{ cal/mol}$, and $E_3 = 30,000 \text{ cal/mol}$. What temperature would you recommend for a single CSTR with a space time of 10 minutes and an entering concentration of A of 0.1 mol/L?

$C_{A0} = 0.1$

$$S_{B/X} = \frac{r_B}{r_X} = \frac{k_2 C_A}{k_1 C_A^{1/2}} = \frac{k_2}{k_1} C_A^{1/2}$$

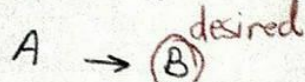
$\tau = 10 \text{ min}$

$$\ln k = \ln A + \frac{E}{T}$$

Low temp.

P6-6

gas phase



Pure A

$$v_0 = 10 \text{ L/min}$$

$$r_X = k_1 C_A^{1/2}$$

$$r_B = k_2 C_A$$

$$r_Y = k_3 C_A^2$$

$$k_1 = 0.004 (\text{mol/L})^{0.5} / \text{min}$$

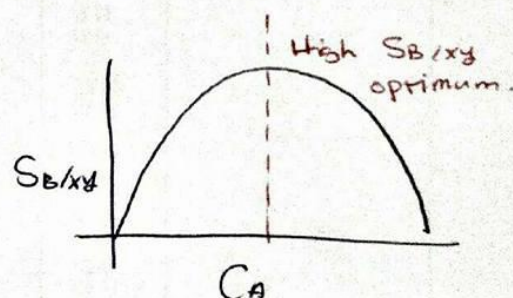
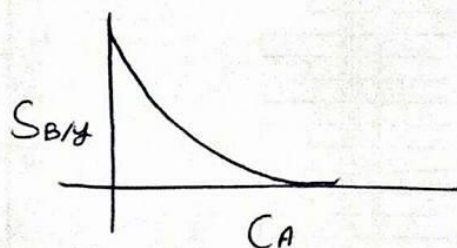
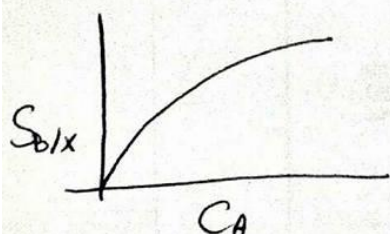
$$k_2 = 0.3 \text{ min}^{-1}$$

$$k_3 = 0.25 \text{ L/mol} \cdot \text{min}$$

$$\textcircled{a} \quad S_{B/X} = \frac{r_B}{r_X} = \frac{k_2 C_A}{k_1 C_A^{0.5}} = \frac{k_2}{k_1} C_A^{0.5} = \frac{0.3}{0.004} C_A^{0.5} = 75 C_A^{0.5}$$

$$S_{B/Y} = \frac{r_B}{r_Y} = \frac{k_2 C_A}{k_3 C_A^2} = \frac{0.3}{0.25} C_A^{-1} = 1.2 C_A^{-1}$$

$$S_{B/X+Y} = \frac{r_B}{r_X + r_Y} = \frac{k_2 C_A}{k_1 C_A^{0.5} + k_3 C_A^2}$$



$$S_{B/X+Y} \text{ max.} = 10 \text{ at } C_A^* = 0.04 \text{ mol/L}$$

↓

So, the CSTR should be used with exist. conc. C_A^*

$$\text{Also, } C_{A0} = \frac{P}{RT} = 0.162 \frac{\text{mol}}{\text{L}}$$

⑥

$$-r_A = r_X + r_B + r_Y = k_1 C_A^{0.5} + k_2 C_A + k_3 C_A^2$$

$$V = \frac{v_0 (C_{A0} - C_A^*)}{-r_A} = \frac{10(0.162 - 0.04)}{k_1 C_A^{*0.5} + k_2 C_A^* + k_3 C_A^{*2}}$$

$$= \frac{10(0.162 - 0.04)}{(0.004)(0.04)^{0.5} + (0.3)(0.04) + (0.25)(0.04)^2}$$

$$V = 92.4 \text{ L}$$

14) How find C_A^* at max. $S_{B/X}$

$$S_{B/X} = \frac{k_2 C_A}{k_1 C_A^{0.5} + k_3 C_A^2}$$

$$\frac{dS_{B/X}}{dC_A} = \frac{k_2 (k_1 C_A^{0.5} + k_3 C_A^2) - k_2 C_A (0.5 k_1 C_A^{-0.5} + 2 k_3 C_A)}{k_1 C_A^{0.5} + k_3 C_A^2}$$

$$0 = (0.3)(0.004 * C_A^{0.5} + 0.25 C_A^2) - (0.3) C_A (0.5 * 0.004 C_A^{-0.5} + 2(0.25) C_A)$$

$$\boxed{C_A^* = 0.04 \text{ mol/L}}$$

$\Rightarrow$ max. selectivity = 10

$$0 = 1.2 \times 10^{-3} C_A^{0.5} + 0.075 C_A^2 - 6 \times 10^{-4} C_A^{0.5} - 0.15 C_A^2$$

$$0 = 6 \times 10^{-4} C_A + 0.075 C_A^2 - 0.15 C_A$$

$$\textcircled{c} \quad \tau = \frac{V}{v_0} = \frac{92}{10} = 9.2 \text{ min}$$

$$V_{\text{STR}} = \frac{F_B - F_{B0}}{r_B}$$

$$V = \frac{v_0 C_B}{r_B}$$

$$\textcircled{1} \quad \tau = \frac{C_B}{r_B}$$

$$9.2 = \frac{C_B}{k_2 C_A^*}$$

$$(9.2)(0.3)(0.8) = C_B^*$$

$$\boxed{C_B^* = 0.11 \text{ mol/L}}$$

$$V = \frac{F_x - F_{x0}}{r_x}$$

$$\tau = \frac{C_x}{k_1 C_A^{0.5}}$$

$$C_x^* = (9.2)(0.004)(0.04)^{0.5}$$

$$\boxed{C_x^* = 0.0074 \frac{\text{mol}}{\text{L}}}$$

$$V = \frac{F_y - F_{y0}}{r_y}$$

$$\tau = \frac{C_y}{k_3 C_A^2}$$

$$C_y^* = (9.2)(0.25)(0.04)^2$$

$$\boxed{C_y^* = 0.0037 \frac{\text{mol}}{\text{L}}}$$

① conversion of A in the 1st reactor

$$X = \frac{C_{A0} - C_A}{C_{A0}} = \frac{0.162 - 0.04}{0.162} = 0.75$$

© CSTR followed by a PFR should be used.
required $X = 0.99$

⇒ for PFR, mole balance: $\frac{dV}{dX} = \frac{F_{A0}}{-r_A}$

$$\int dV = \int \frac{F_{A0}}{-r_A} dX$$

$$= \frac{V_0 C_{A0}}{k_1 C_{A0}^{0.5} + k_2 C_A + k_3 C_A^2} \int_{0.75}^{0.99} dX$$

~~$$V = \frac{(10)(0.162)}{(0.004)(0.04)^{0.5} + (0.3)(0.04) + (0.25)(0.04)^2} \int_{0.75}^{0.99} dX$$~~

~~$$V = (122.73)(0.99 - 0.75)$$~~

Assume isothermal isobaric operation

and we know $\boxed{E = \gamma S = 0}$

⇒ $\boxed{V = V_0}$

⇒ $C_A = C_{A0}(1-X)_{0.99} \Rightarrow C_A = 1.62 \times 10^{-3}$

$$V = (10)(0.162) \int_{0.75}^{0.99} \frac{dX}{(0.004)(\underbrace{C_{A0}}_{0.162 \times 10^{-3}})^{0.5}(1-X)^{0.5} + (0.3)(0.162)(1-X) + (0.25)(0.162)^2(1-X)^2}$$

$\boxed{V = 92 \text{ L}}$

Partner (1) Name: Samir, 2009, 10 Partner (2) Name: _____

Partner (1) ID #: _____ Partner (2) ID #: _____

Example: PBR with Heat Exchange and Pressure Drop

The elementary reversible reaction $A + B \rightleftharpoons C$ is carried out in a PBR with constant coolant temperature (T_c). We want to determine both the conversion and temperature profiles.

Write a Polymath program to plot X and T vs. W .

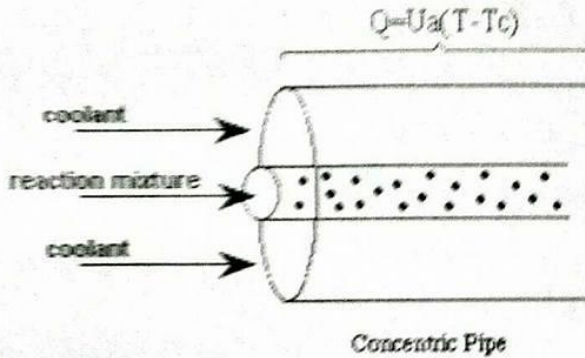
$$v_0 = 50 \text{ L/s}$$

$$F_{A0} = 5 \text{ mol/s}$$

$$F_{B0} = F_{A0}$$

$$F_I = F_{A0}$$

$$T_0 = 325 \text{ K}$$



$$E = 25 \text{ kcal/mol}$$

$$\Delta H_{Rx} = -20 \text{ kcal/mol}$$

$$k = 0.004 \frac{\text{dm}^3}{\text{kg} \cdot \text{mol} \cdot \text{s}} @ 310 \text{ K}$$

$$K_C = 1000 @ 303 \text{ K}$$

$$\alpha = 0.0002 / \text{kg}$$

$$W = 2500 \text{ kg}$$

$$C_{Ps} = C_{Pc} = C_{Pi} = 20 \text{ cal/mol/K}$$

$$C_{Pj} = 40 \text{ cal/mol/K}$$

$$\frac{Ua}{\rho_s} = 0.5 \frac{\text{cal}}{\text{kg} \cdot \text{s} \cdot \text{K}}$$

$$T_s = 325 \text{ K}$$

Solution:

1) Mole Balance:

$$\frac{dF_A}{dW} = -r_A$$

$$F_{A0} = 5 \text{ mol/s}$$

2) Rate Law:

$$-r_A = k \left(C_A C_B - \frac{C_C}{K_C} \right)$$

$$k = k_1 \exp \left(\frac{-E}{R} \left(\frac{1}{T} - \frac{1}{T_1} \right) \right)$$

$$k_1 = 0.004 \text{ dm}^3 / \text{mol} \cdot \text{s}$$

$$T_1 = 310 \text{ K}$$

$$E = 25,000 \text{ cal/mol}, \quad R = 1.987 \frac{\text{cal}}{\text{mol} \cdot \text{K}}$$

$$K_C = k_{c2} \exp \left(\frac{-\Delta H_{Rx}}{R} \left(\frac{1}{T} - \frac{1}{T_1} \right) \right)$$

$$k_{c2} = 1000$$

$$T_2 = 303 \text{ K}$$

$$\Delta H_{Rx} = 20,000 \text{ cal/mol}$$

$$\Delta C_p = 0$$

$$\Delta H_{Rx} \approx 0$$

$$T \approx 325 \text{ K}$$

$$C_A = \frac{C_{A0}(1-x)}{1+\epsilon x} y \frac{T_0}{T}$$

$$C_B = \frac{C_{A0}(1-x)}{1+\epsilon x} y \frac{T_0}{T}$$

$$C_C = \frac{C_{A0}x}{1+\epsilon x} y \frac{T_0}{T}$$

$$C_{A0} = \frac{5}{50} = 0.1 \text{ mol/L}$$

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

$$T_0 = 325 \text{ K}$$

$$\frac{dy}{dw} = \frac{-\alpha}{2y} (1 + \epsilon x) \frac{T_0}{T} \quad \text{NOT const Temp. } \epsilon \neq 0$$

$$\alpha = 0.0002 \text{ kg}^{-1}$$

For a packed bed reactor ($dw = S_b dv$) where $S_b = \text{densing at bulk}$

The Energy
Balance
for
PBR Reactor:

$$\frac{dT}{dw} = \frac{U_a}{S_b} \frac{(T_a - T) + r_A' \Delta H_{rx}}{F_{A0} (\sum \Theta_i C_{pi} + \Delta C_p x)}$$

$$\frac{U_a}{S_b} = 0.5 \frac{\text{cal}}{\text{kg} \cdot \text{s} \cdot \text{K}}$$

$$T_a = 325 \text{ K}$$

$$\textcircled{a} \quad w = 0, \quad x = 0, \quad y = 1$$

$$T = 325 \text{ K}$$

$$w_F = 2500 \text{ kg}$$

$$\begin{aligned} \sum \Theta_i C_{pi} &= C_{pA} + \Theta_B C_{pB} + \Theta_I C_{pI} \\ &= 20 + (1)(20) + (1)(40) \\ &= 80 \frac{\text{cal}}{\text{mol} \cdot \text{K}} \end{aligned}$$

by Polymath solve $\boxed{x}$

(0905421) Chemical Reaction Engineering I

In-Class Assessment # 25 (Chapter 8)

Partner (1) Name: Osama Al-Hamoud Partner (2) Name: _____

Identity (1) #: _____ Identity (2) #: _____

P8-5 CSTR with Heat Effect

The endothermic (liquid-phase) elementary reaction $A + B \rightarrow 2C$ proceeds, substantially, to completion in a single steam-jacketed, continuous-stirred reactor. From the following data, calculate the steady-state reactor temperature:

Reactor volume: 125 gal Steam jacket area: 10 ft² Agitator shaft horsepower: 25 hp
Jacket steam: 150 psig (365.9 °F saturation temperature)
Overall heat-transfer coefficient of jacket, U : 150 Btu/h.ft².°F
Heat of reaction, $\Delta H_{Rx}^0 = +20,000$ Btu/lb mol of A (independent of temperature) $\Rightarrow \Delta C_p = 0$

Component	A	B	C
Feed (lbmol/hr)	10.0	10.0	0
Feed temperature (°F)	80	80	-
Specific heat (Btu/lb mol. °F)	51.0	44.0	47.5
Molecular weight	128	94	222
Density (lb/ft ³)	63.0	67.2	65.0

$$X_{EB} = \frac{\frac{UA}{F_{A0}} (T - T_a) + \sum \Theta C_{pi} (T - T_0)}{-\Delta H_{Rx}} \Rightarrow 1 = \frac{\left(\frac{150 \text{ Btu}}{\text{h.ft}^2 \cdot \text{F}} \right) \left(\frac{10 \text{ ft}^2}{10 \text{ lbmol/h}} \right) (T - 365.9) + \frac{-63525 \text{ Btu}}{\text{h}}}{95(T - 80)}$$

But there is $\dot{W}_s$

$$\dot{Q} = UA (T_a - T)$$

$\dot{Q} - \dot{W}_s \Rightarrow$ NOT Neglect for shaft work

$$\dot{W}_s = -25 \text{ hp} = -63525 \text{ Btu/h}$$

done on the system.

$$\dot{Q} = UA (T - T_a) + \dot{W}_s$$

Solution:

$$V = \frac{F_{A0} X}{-r_A}$$

$$-r_A = k C_A C_B$$

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

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

المعادلة تبدأ من هنا
تكون درجة الحرارة المستقر

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

$$k = k_1 \exp \left(\frac{-E}{R} \left(\frac{1}{T} - \frac{1}{T_1} \right) \right)$$

$$C_p = \sum \text{Prod.} - \sum \text{Reactants}$$

$$\Delta C_p = 0$$

$$\sum \Theta_i C_{pi} = C_{pA} + (1) C_{pB} = 95 \frac{\text{Btu}}{\text{lbmol} \cdot \text{F}}$$

$$-20,000 \text{ Btu/lbmol}$$

(0905421) Chemical Reaction Engineering I

In-Class Assessment # 23 (Chapter 8)

Partner (1) Name: _____

Partner (2) Name: _____

Partner (1) ID #: _____

Partner (2) ID #: _____

P8-6 The elementary irreversible organic liquid-phase reaction $A + B \rightarrow C$ is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters at 27°C , and the volumetric flow rate is $2 \text{ dm}^3/\text{s}$ and $C_{A0} = 0.1 \text{ kmol/m}^3$.

Additional information:

At reference Temp.
 $H_A^\circ(273 \text{ K}) = -20 \text{ kcal/mol}$

$C_{pA} = C_{pB} = 15 \text{ cal/(mol.K)}$

$k = 0.01 \text{ L/(mol.s)}$ at 300 K

$H_B^\circ(273 \text{ K}) = -15 \text{ kcal/mol}$

$C_{pC} = 30 \text{ cal/(mol.K)}$

$E = 10,000 \text{ cal/mol}$

$H_C^\circ(273 \text{ K}) = -41 \text{ kcal/mol}$

(a) Calculate the PFR and CSTR volumes necessary to achieve 85% conversion. What are the reasons for the differences?

CSTR

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

liquid ✓

elementary $A+B \rightarrow C$ ✓

adiabatic ✓

$F_{A0} = F_{B0}$

$T_0 = 27^\circ\text{C} = 300 \text{ K}$

$v_0 = 2 \text{ dm}^3/\text{s}$

$C_{A0} = 0.1 \text{ kmol/m}^3$
 $= 0.1 \text{ mol/dm}^3$

$x = 85\%$

① PFR

mol balance: $V = F_{A0} \int_0^x \frac{dx}{-r_A}$

rate law: $-r_A = k C_A C_B$

$k = k_1 \exp\left(-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_1}\right)\right)$

$k_1 = 0.01 \text{ L/mol.s}$ @ $T_1 = 300 \text{ K}$

stoich: $C_A = C_{A0}(1-x)$

$C_B = C_{A0}(\theta + \nu_B x)$

$= C_{A0}(1-x)$

$\Rightarrow -r_A = k C_{A0}^2 (1-x)^2$

Note: You can use 'Simpson's $\frac{3}{8}$ rule' if numerical integration is needed:

$$\int_{x_0}^{x_3} f(x) dx = \frac{3h}{8} [f_0 + 3f_1 + 3f_2 + f_3]$$

$$h = \frac{x_3 - x_0}{3}$$

① $V = F_{A0} \int_0^{0.85} \frac{dx}{k \exp\left(-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_1}\right)\right) C_{A0}^2 (1-x)^2}$

$\Delta C_p = C_{pC} - C_{pB} - C_{pA}$
 $= 30 - 15 - 15 = 0$

energy balance $\Rightarrow T = T_0 + \frac{-\Delta H_{Rx} \cdot X}{\sum \theta_i C_{pi}}$

$\Delta H_{Rx} = H_C - H_B - H_A$

$= -6 \text{ kcal/mol}$

$= -6000 \text{ cal/mol}$

$T = 300 + \frac{6000 X}{C_{pA} + \theta C_{pB}} = \frac{6000 X + 300}{15 + (1)(15)}$

$T = 300 + \frac{6000 X}{30}$

$T = 300 + 200 X$

① 3 words

exothermic $\uparrow T \uparrow X$

- (b) What is the maximum inlet temperature one could have so that the boiling point of the liquid (550 K) would not be exceeded even for complete conversion?

$$T = T_0 + 200X$$

$\parallel$ $\parallel$
 550 1

$T_0 = 350 \text{ K}$ $X=1$

- (d) Calculate the conversion that can be achieved in one 500-dm³ CSTR and in two 250-dm³ CSTRs in series.

$X = ?$ $V_{\text{CSTR}} = 500 \text{ dm}^3$

$$V = \frac{F_{A0} X}{k C_{A0}^2 (1-X)^2}$$

$\downarrow$
 $k_{\text{exp}} \left(\frac{-E}{R} \left(\frac{1}{T} - \frac{1}{T_1} \right) \right)$
 $\downarrow$ $\downarrow$ $\downarrow$
 0.01 300 + 100X 300

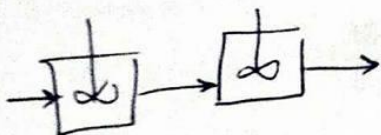
by trial & error

$\left[\begin{array}{l} X=0.5 \\ V=60 \text{ L} \end{array} \right.$

$\left[\begin{array}{l} X=0.9 \\ V=333 \text{ L} \end{array} \right.$

$\left[\begin{array}{l} X=0.93 \\ V=618 \text{ L} \end{array} \right.$

$\left[\begin{array}{l} X=0.921 \\ V=499 \text{ L} \end{array} \right.$



$V_1 = 250 = \frac{0.2 X_1}{(k(0.1))^2 (1-X_1)^2}$

$0.87 \rightarrow 217 \text{ L}$

$X_1 = 0.882$

$250 = V_2 = \frac{F_{A0} (X_2 - 0.882)}{k C_{A0}^2 (1-X_2)^2}$

$X_2 = 0.945 \rightarrow V_2 = 134 \text{ L}$

$X_2 = 0.98 \rightarrow V_2 = 600 \text{ L}$

$X_2 = 0.967$

$X=0.7 \Rightarrow V=74.8$

$X=0.8 \Rightarrow V=116.9$

$X=0.9 \Rightarrow V=338$

$V=250 \text{ L} \Rightarrow X_1 = 0.862$

$0.862 \rightarrow 217 \text{ L}$

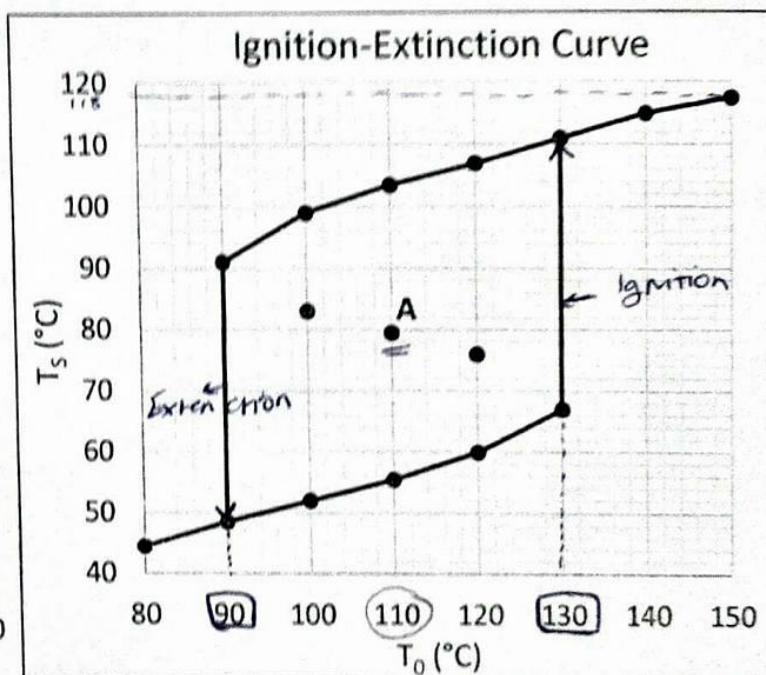
Partner (2) Name: _____

Identity (2) #: _____

Ambient temperature, $T_a = 300$ K

90%

130°C



Is this a locally stable steady state point? Why? NO, it's ~~not~~ ~~unstable~~ ~~stable~~ ~~state~~
an Un-stable, because do not return to it if there is a temp. Pulse.

118°

(e) Suppose that the fluid is now heated to 140 °C and then cooled to 120 °C, where it remains. What will be the reactor temperature and conversion?

(0905421) Chemical Reaction Engineering I

In-Class Assessment # 27 (Chapter 8)

Partner (1) Name: Partner (2) Name:

Identity (1) #: Identity (2) #:

P8-13 The reaction $A + B \rightleftharpoons C + D$ is carried out adiabatically in a series of staged packed-bed reactors with inter-stage cooling. The lowest temperature to which the reactant stream may be cooled is 27 °C. The feed is equal molar in A and B and the catalyst weight in each reactor is sufficient to achieve 99.9% of the equilibrium conversion. The feed enters at 27 °C. If four reactors and three coolers are available, what conversion may be achieved?

$$T = 27 + 273 = 300 \text{ K}$$

$$X_e = 0.999$$

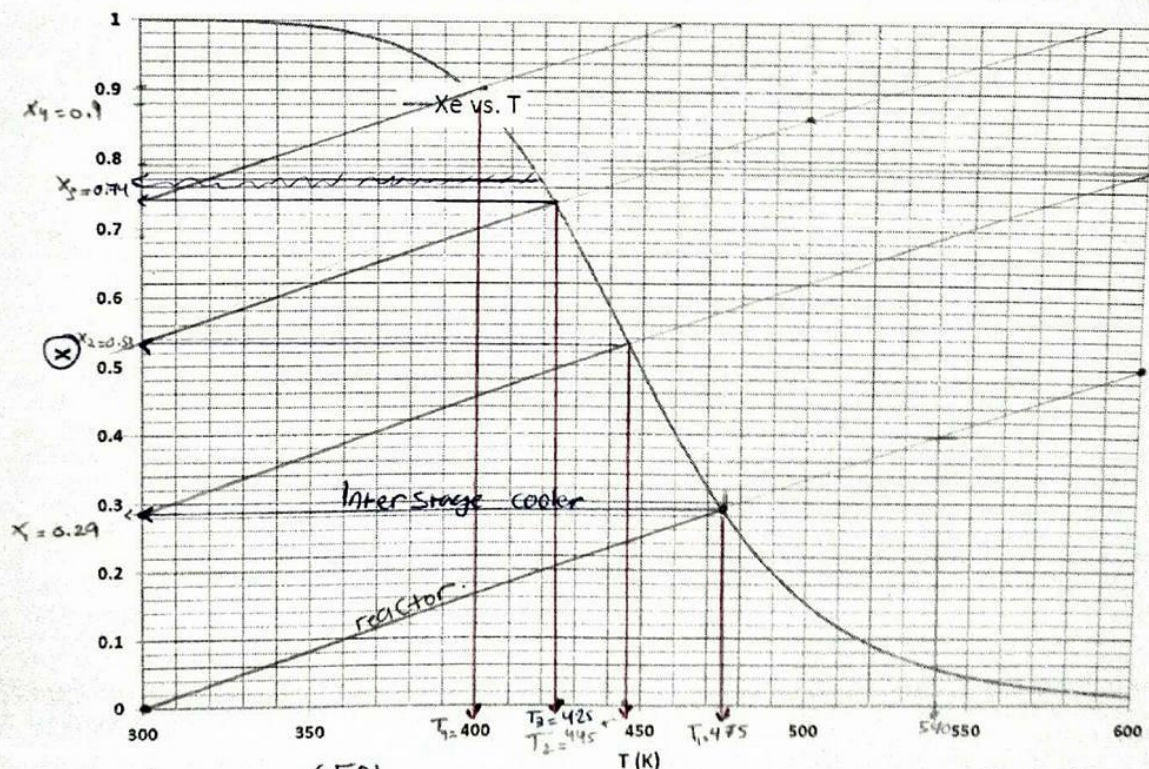
Additional information:

$$\Delta H_{Rx} = -30,000 \text{ cal/mol A} \quad C_{PA} = C_{PB} = C_{PC} = C_{PD} = 25 \text{ cal/mol.K}$$

$$K_e (50 \text{ °C}) = 50,000 \quad F_{A0} = 10 \text{ mol A/min}$$

Solution:

① Prepare a plot of equilibrium conversion as a function of temperature.



② Use the adiabatic energy balance equation to find the relation between T and X.

$$T = T_0 + \frac{-\Delta H_{Rx} \cdot X}{\sum \theta_i C_{Pi}} = 300 + \frac{30,000X}{C_{PA} + C_{PB}} \rightarrow T = 300 + 600X \rightarrow (T-300) = 600(X-0)$$

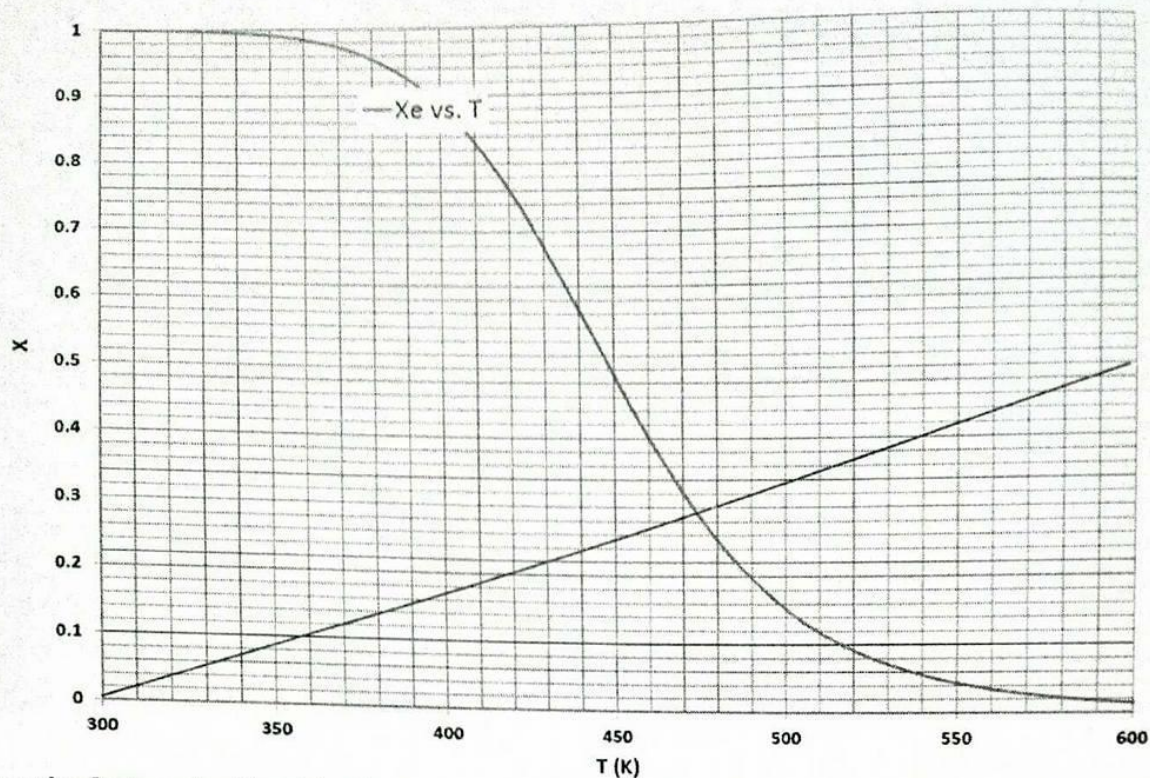
③ Draw the line that represents the first reactor on the equilibrium plot:

(It's a straight line that passes through the 2 points (300, 0) and (600, 0.5))

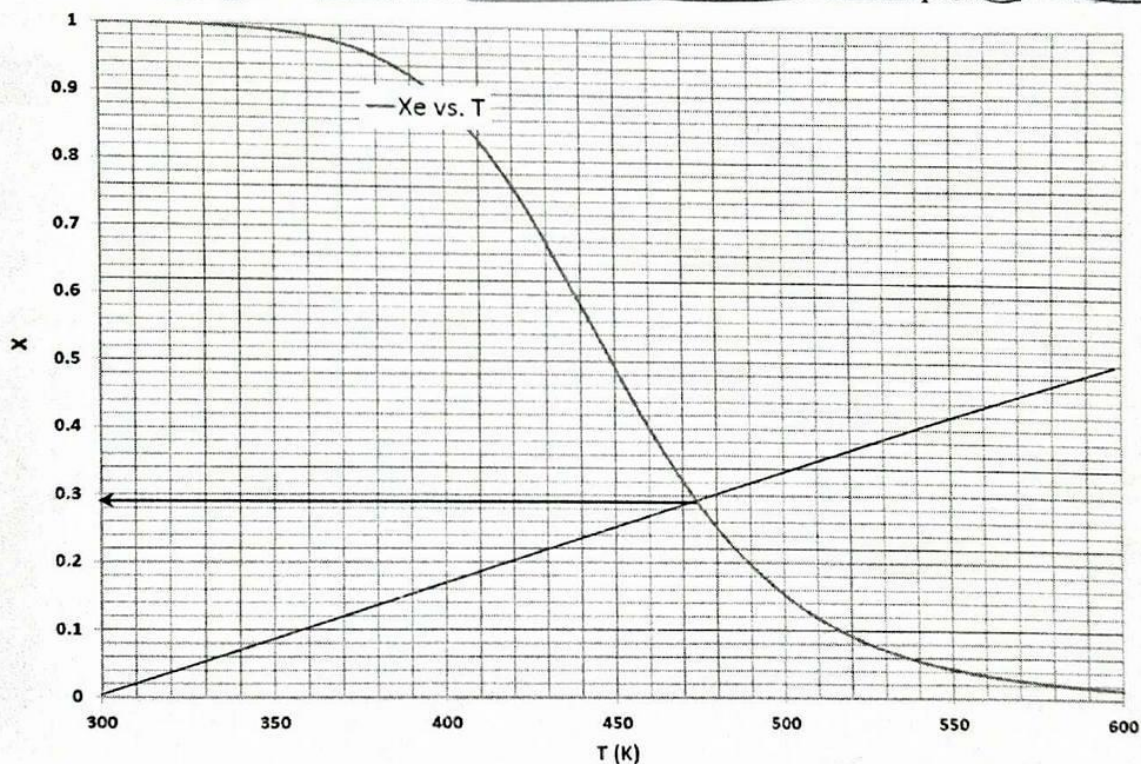
$$X=0 \rightarrow T=300$$

$$X=0.5 \rightarrow T=600$$

From the plot below, we see that $X_1 = 0.29$ and $T_1 = 475 \text{ K}$



- ④ Draw the first cooler line, it's a horizontal line from the first reactor exit temperature to 300 K.



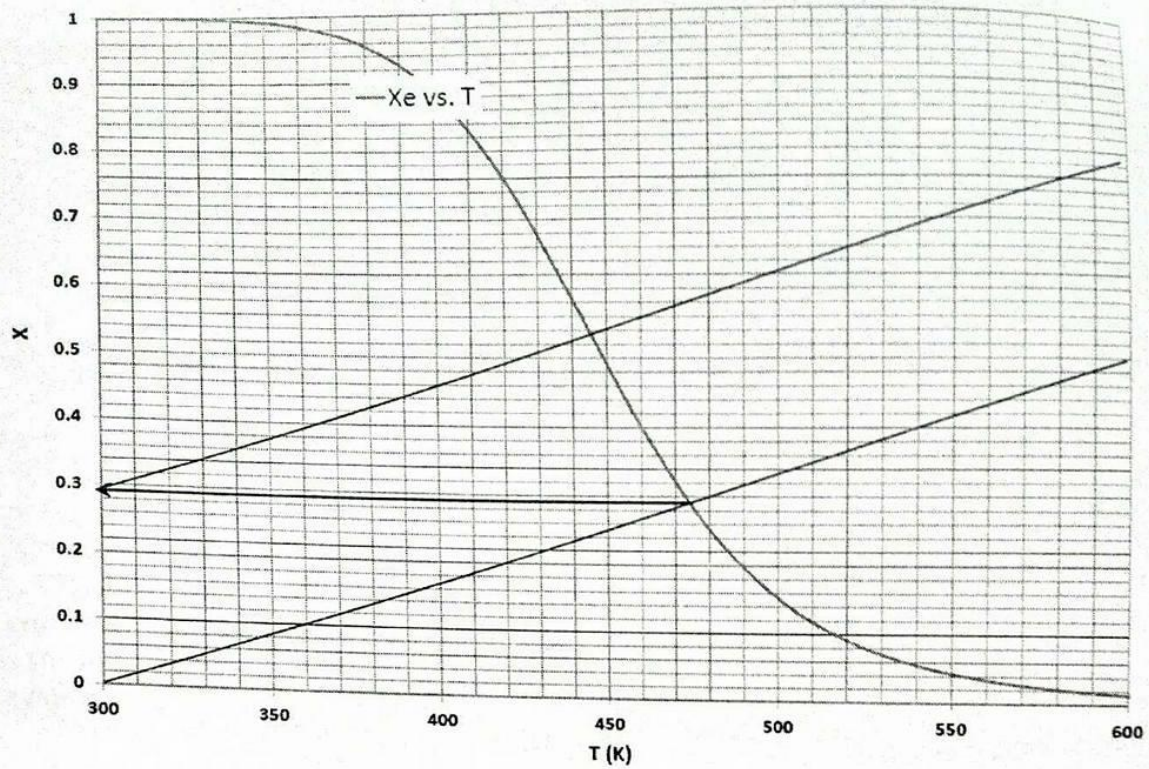
- ⑤ Draw the line that represents the second reactor on the equilibrium plot; it's parallel to the first reactor but starts from the point (300, 0.29).

You can also draw it by using the adiabatic equation $T = 300 + 600X$ but after remembering that this equation is originally $(T - 300) = 600(X - 0)$, so now it can be used after being modified to $(T_2 - 300) = 600(X_2 - X_1)$

⇒ It's a straight line that passes through the 2 points: (300, 0.29) and (600, 0.79)

From the plot below, we see that $X_2 = 0.53$ and $T_2 = 445 \text{ K}$.

$$\Rightarrow (600 - 300) = 600 (X_2 - 0.29) \Rightarrow X_2 = 0.79$$



- 6- Now repeat steps 4 and 5 two times; draw the second cooler horizontal line, the third reactor adiabatic line ($X_3 = 0.74$ and $T_3 = 425$ K), the third cooler horizontal line, and the fourth reactor adiabatic line ($X_4 = 0.90$ and $T_4 = 400$ K).

