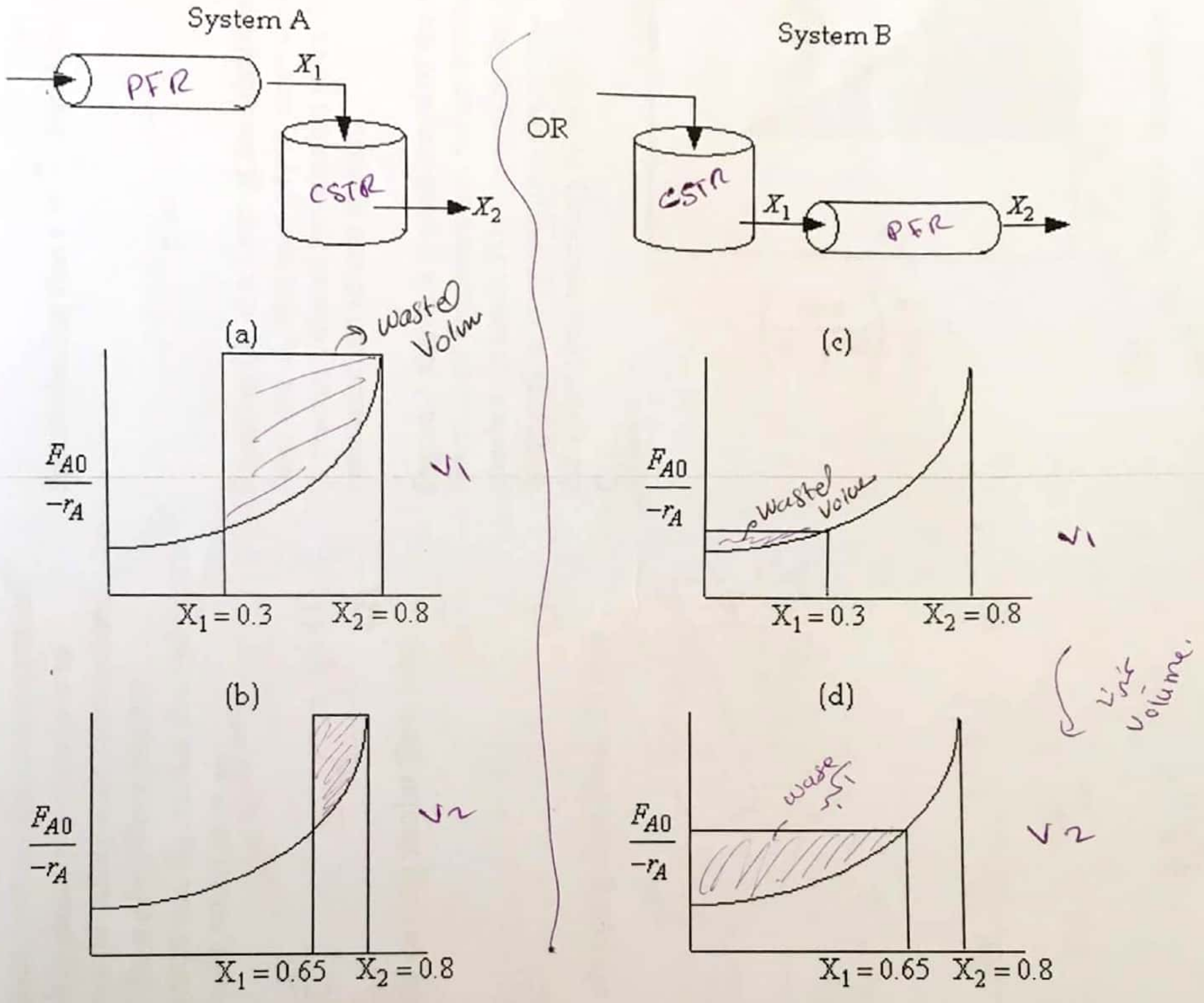
The University of Jordan
School of Engineering
Chemical Engineering Department

(0905421) Chemical Reaction Engineering I	**In-Class Assessment # 6 (Chapter 2)**
Partner (1) Name: Sarah.	**Partner (2) Name:**
Identity (1) #:	**Identity (2) #:**

Self-Test



Q1. Which system is most efficient for an intermediate conversion of (0.3)? a OR [✓ c]

Q2. Which system is most efficient for an intermediate conversion of (0.65)? [✓ b] waste volume أقل efficient أكثر

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

system B, with intermediate conversion [✓ c]

عشان overall conversion

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(0905421) Chemical Reaction Engineering I	**In-Class Assessment # 5 (Chapter 2)**
Partner (1) Name: Sarah.	**Partner (2) Name:**
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 → 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:

$v = 1\ L/s$

$-r_A$	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 maximum conversion that can be achieved with these two reactors connected in series?

① CSTR → ② PFR

ثاني شيء

$x \times 0.4$

$\textcircled{x}$	0.4
V	480

x	0.6
V	288

0.5

132

تقريباً اكبر من 0.5

CSTR ≈ $X \leq 0.57$

X	0.6	0.5
V	504	288

① PFR → CSTR

100L 400L

اولوياتها

X	0.2	0.3
V	48	108 ≈ 100L

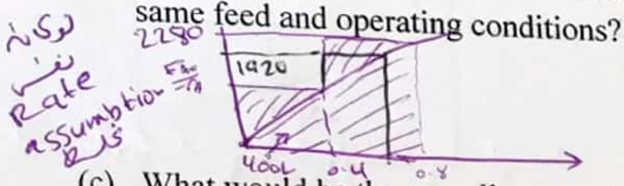
→ تقريباً

PFR → 30% conv

حجم الغرفة الاولى

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

لو كانت نفس Rate assumption



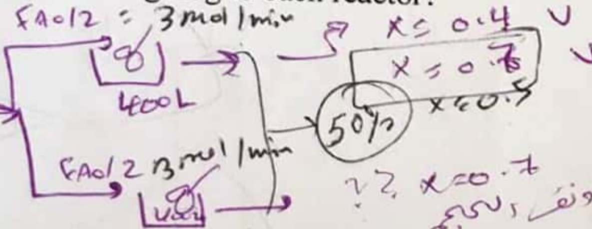
$V_{0.4 \to 0.8} = 2280 \times (0.8 - 0.4)$
$\approx 0.8 = 912L$ Ⓧ كبير rate of rxn
overall conversion ?

$V_{0.4 \to 0.65} = 1920\ (0.65 - 0.4)$
$= 380\ L$

اكبر من $x = 0.4$

(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?

Series اعلى conversion من FA0



$X \leq 0.4$ $V = 245.8L$

$X = 0.7$ $V = \cancel{419.6}\ L$ ✓

$X \leq 0.5$ $V = 425\ 734.3L$

?? $x = 0.7$

$x = 0.4$

Reactor ← تفاعل بزيد conv

residuns time

$\tau = \frac{V}{v_0}$

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

? $P_{A0} v_0 = F_{A0} RT$ → stream flow rate
volumetric flow rate. reactor.

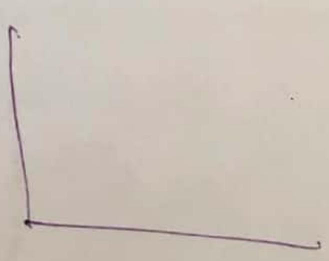
قل ↓

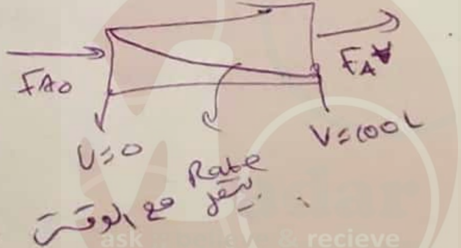
$V = \frac{F_{A0}\ X^{\uparrow}}{-r_A}$

conversion increase.
$X_2 = 10X_1$ →

$\tau = \frac{V}{v_0}$

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





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(0905421) Chemical Reaction Engineering I	**In-Class Assessment # 4 (Chapter 2)**
Partner (1) Name: Sarah.	**Partner (2) Name:**
Identity (1) #:	**Identity (2) #:**

The gas-phase reaction A + B → 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. L/s

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

[illegible] convert

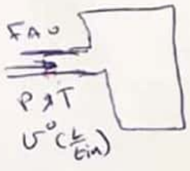
×60

mol/s

CSTR

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

$$V = \frac{F_{A0}(X_{out} - X_{in})}{-r_{A(out)}}$$



$$V = \frac{F_{A0}X}{-r_A} = \frac{0.1 \times 0.7}{0.0028\ \frac{mol}{min.L}}$$

$= 1468L$

$F_{A0} = 0.41\left(\frac{PV}{RT}\right)$ mol

$$F_{A0} = \frac{P_{A0}\upsilon_0}{RT}$$

$P_{A0} = y_A P_{tot}$

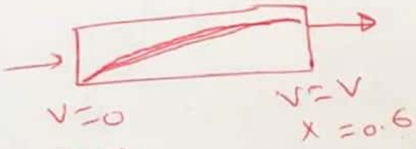
(b) What is the volume of a single tubular reactor necessary to achieve 60% conversion?

PFR

$$F_{A0} = \frac{0.41 \times 10 \times 1L}{0.08206 \times 500\ K}$$

$F_{A0} = 0.1$ mo

$$V = \int_0^X \frac{F_{A0}\,dX}{-r_A}$$



$$F_{A0}\int_0^X \frac{dX}{-r_A}$$

X is not constant

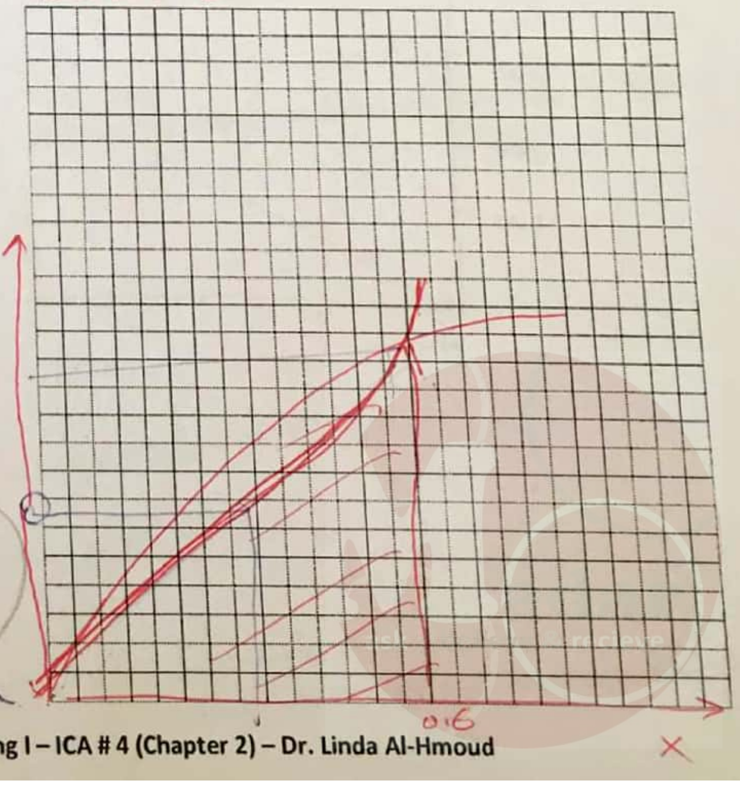
~~#~~ of mole → F_0 (flowrate) is not constant

$-r_A$ تقل مع X

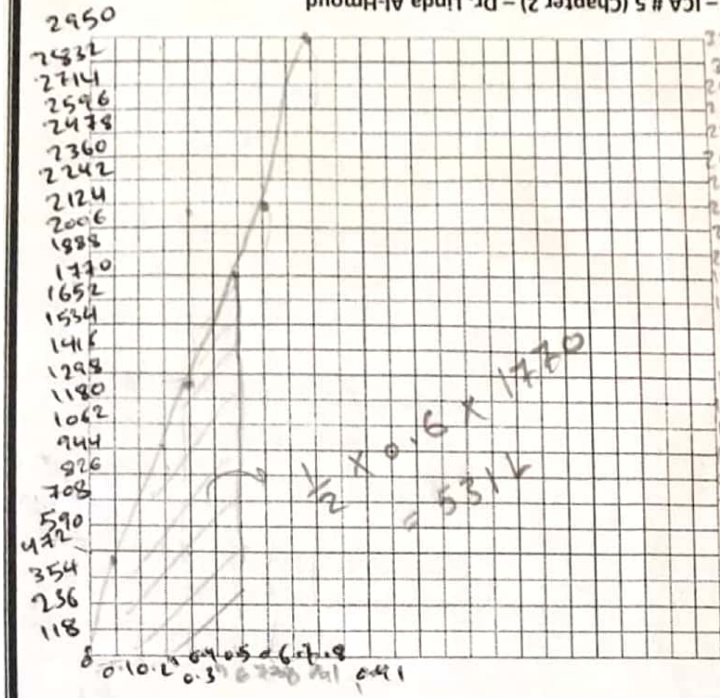
$-\frac{1}{r_A}$ تزيد مع X

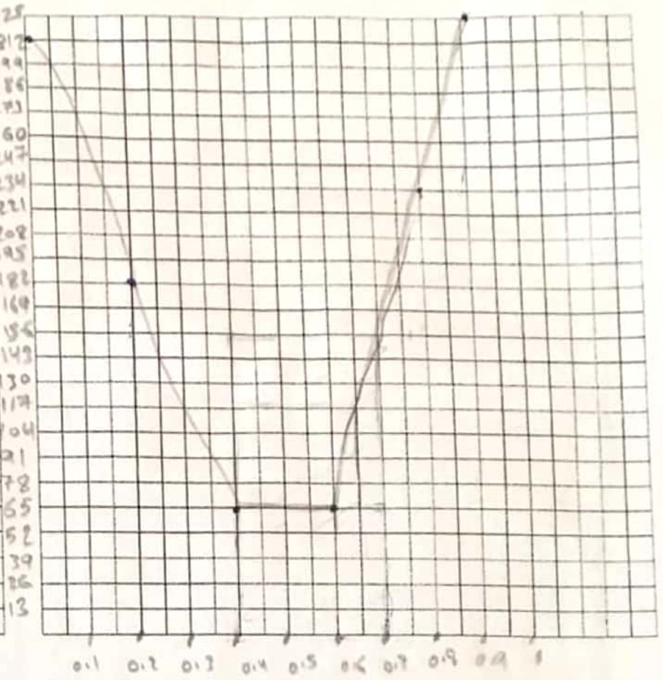
$\frac{1}{-r_A}$ F_0

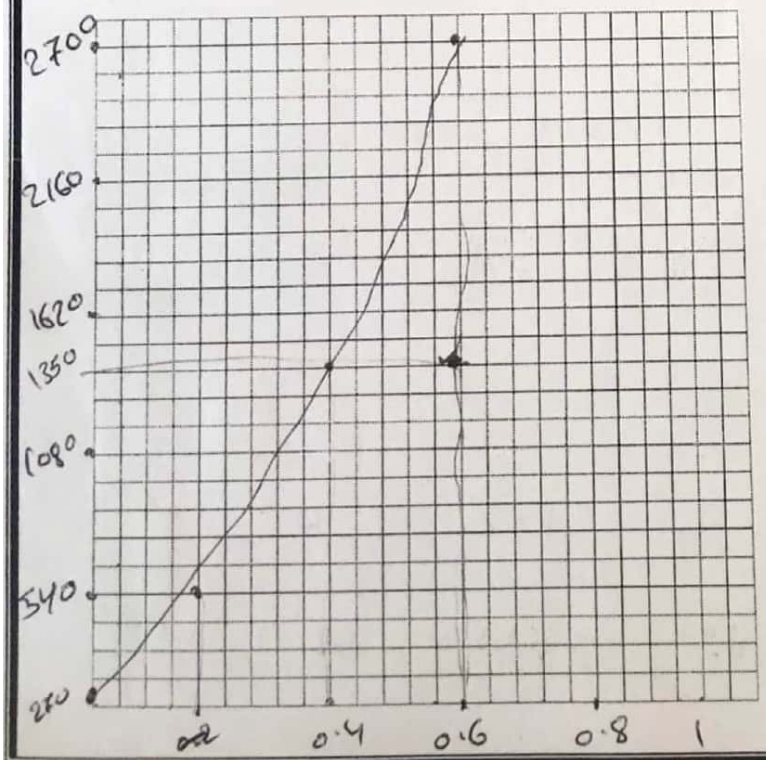
?



V = FAo Aera under the curve


2950
2832
2714
2596
2478
2360
2242
2124
2006
1888
1770
1652
1534
1416
1298
1180
1062
944
826
708
590
472
354
236
118
0
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8
$\frac{1}{2} \times 0.6 \times 1770$
$= 531$


225
212
299
286
273
260
247
234
221
208
195
182
169
156
143
130
117
104
91
78
65
52
39
26
13
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1


2700
2160
1620
1350
1080
540
270
0.2
0.4
0.6
0.8
1

Levenspiel Plots in Terms of Conversion

concentration

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 $\upsilon = \upsilon_0$.

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

→ mole Balance

$F_{A0} \rightarrow \square \rightarrow F_A$

$$F_{A0} = \upsilon_0 C_{A0} \quad (2)$$

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

in - out / in

$$X = \frac{F_{A0} - F_A}{F_{A0}} = 1 - \frac{F_A}{F_{A0}} \quad (3)$$

For the special case when $\upsilon = \upsilon_0$, plugging Equation (2) into Equation (3), we get

constant volume flowrate

in = out

$$X = \frac{\cancel{\upsilon_0} C_{A0} - \overset{=\upsilon_0}{\upsilon} C_A}{C_{A0}\cancel{\upsilon_0}} \quad (4)$$

$$\boxed{X = \frac{C_{A0} - C_A}{C_{A0}}}$$

$$1 - \frac{\cancel{\upsilon} C_A}{\cancel{\upsilon_0} C_{A0}}$$

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

نغير الحدود, للتكامل

Differentiating Equation (4) yields

$\upsilon = \upsilon_0$

$$dX = \frac{\cancel{\upsilon}}{\cancel{\upsilon_0} C_{A0}} \partial C_A \quad (5)$$

$$\partial x = \frac{-1}{C_{A0}} \partial C_A$$

And substituting in Equation (1):

$$\frac{\partial x}{\partial C_A} = \frac{-1}{C_{A0}}$$

$$V = F_{A0}\int_{C_{A0}}^{C_A} \frac{-1}{C_{A0} r_A} \partial C_A = -\frac{F_{A0}}{C_{A0}} \int \frac{\partial C_A}{-r_A} \quad (6)$$

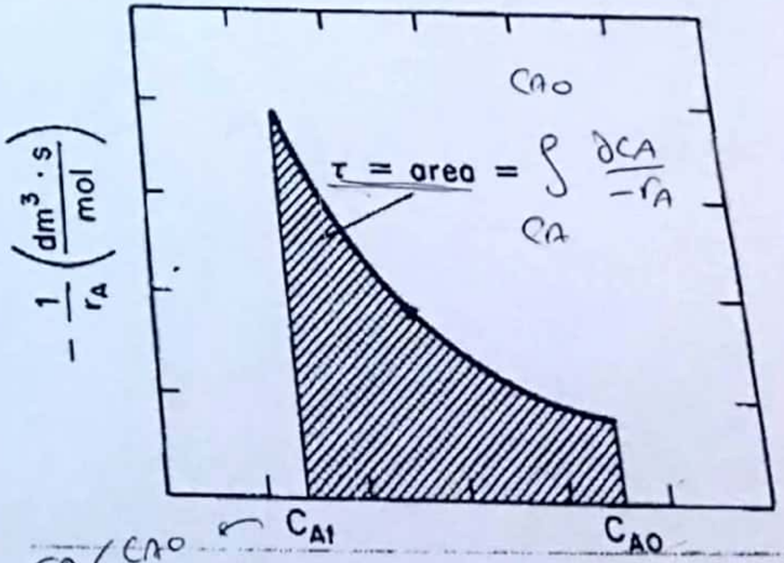
Remembering that $\tau = \frac{V}{\upsilon_0}$, Equation (6) can be rewritten as:

$$= -\upsilon_0 \int_{C_{A0}}^{C_A} \frac{\partial C_A}{-r_A}$$

$$\tau = \frac{-\cancel{\upsilon_0} \int \frac{\partial C_A}{-r_A}}{\cancel{\upsilon_0}} = \int_{C_A}^{C_{A0}} \frac{\partial C_A}{-r_A}$$

Equation (7) is a form of the design equation for constant volumetric flow rate υ_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}.



$C_A < C_{A0}$

تقل conc مع ا ناقصة

Figure 1 Determining the space time, τ.

ssessment # 7 (Chapter 3)

Partner (1) Name: Sarah **Partner (2) Name:** ____________

Identity (1) #: ____________ **Identity (2) #:** ____________

Data on the tenebrionid beetle whose body mass is 3.3 g show that it can push a 35-g ball of dung at 6.5 cm/s at 27 °C, 13 cm/s at 37 °C, and 18 cm/s at 40 °C. How fast can it push dung at 41.5 °C?

Hint: the behavior of the beetle can be modeled by the Arrhenius equation.

T	27 C° 300	37 C° 310	40 C° 313	41.5C° 314.5
V $\xrightarrow{}$ $\boxed{K}$	6.5 cm/s	13 cm/s	18 cm/s	??
1/T	0.003	0.00322	0.00319	0.00318
ln k	~~8.314~~ 1.87	2.5649	2.89	??

$\boxed{24\ \text{cm/s}}$

$$\ln k = \ln \underset{?}{A} - \frac{E}{RT}$$ in kelvin

$$\frac{E}{R} = \cancel{2.74\times10^{3}\,K}\ \cancel{300\,K}\ 8600\,K$$

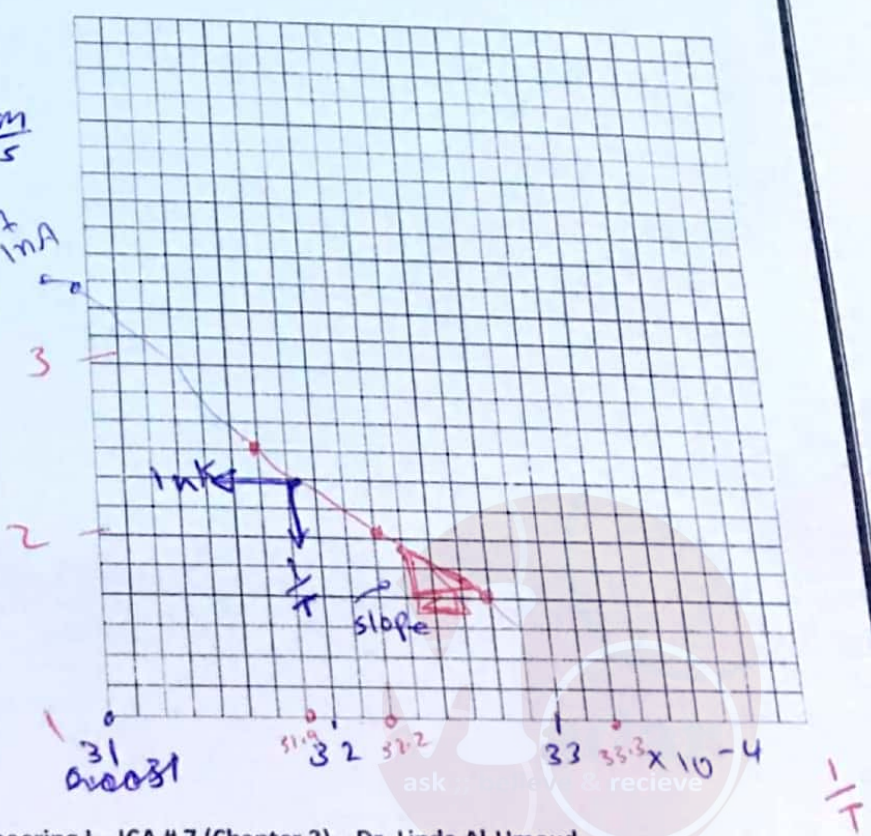
lnk

~~A ×10~~ cm/s

$$A = 1.8\times10^{13}\ \frac{cm}{s}$$

slope
منه الرسمة .
طلع منه
Table
اذا كانت
الشغلة
كان line
بنزبط

not A
OR lnA
لانو
scale
ما بلش من
الصفر



P3-16$_B$ Calculate the equilibrium conversion and concentrations for each of the following reactions. constant volum.

(a) The liquid-phase reaction

$$A + B \rightleftarrows C$$

$$\Theta_B = \frac{C_{B0}}{C_{A0}} = \frac{2}{2} = 1$$

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

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

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

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

$$C_C = C_{A0}(0+X)$$

$$0 = k\left(C_{A0}^2(1-X_e)^2 - \frac{C_{A0}X_e}{K_C}\right)$$

$$C_{A0}(1-X_e)^2 = \frac{X_e}{K_C}$$

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

$$\boxed{X_e = 0.95}$$

(b) The gas-phase reaction

$$A \leftrightarrow 3C$$

$P = P_0$ (Isobaric), $y_{A0} = 1$

carried out in a flow reactor with no pressure drop. Pure A enters at a temperature of $\underset{T_0}{400\text{ K}}$ and $\underset{P_0}{10\text{ atm}}$. At this temperature, $K_C = 0.25(\text{dm}^3/\text{mol})^2$. Assume Isothermal $T = T_0$

Assume

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

$$C_{A0} = \frac{10 \times 1}{0.08206 \times 400} = 0.305\ \frac{\text{mol}}{\text{L}}$$

$$\varepsilon = y_{A0}\,\delta$$

$$\varepsilon = (1)(3-1) = 2$$

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

$$C_C = C_{A0}\frac{(0+3X)}{1+\varepsilon X}$$

$$0 = k\left(\frac{C_{A0}(1-X)}{1+2X} - \left(3\frac{C_{A0}X}{1+2X}\right)^3 \frac{1}{K}\right)$$

$$1 - X_e = \frac{3\,\underset{0.305}{C_{A0}^2}\,X_e^3}{(1+2X_e)^2\,(0.25)}$$

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

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

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(0905421) Chemical Reaction Engineering I **In-Class Assessment # 11 (Chapter 3)**

Partner (1) Name: ____________ **Partner (2) Name:** ____________

Identity (1) #: $-r_A = \frac{k C_{A0}^{3/2} (1-X)^{3/2}}{\sqrt{2}\,(1-X/3)^{3/2}}$ **Identity (2) #:** ____________

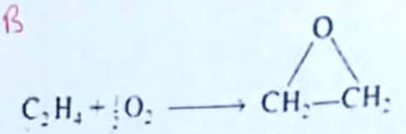
P3-11$_A$ Set up a stoichiometric table for the each of the following reactions and express the concentration of each species in the reaction as a function of conversion evaluating all constants (e.g. ε. Θ). Then, assume the reaction follows an elementary rate law, and write the reaction rate solely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

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

Feed : 1mol A + 0.5 mol B

stoicumetry feed
هاد بيعني ?
stoic umeth
اذا الاثنين
limiting
Read-ant

Flowsystem



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

$A + \frac{1}{2} B \rightarrow C$

species	symbool	Entring	Charpe	leaving
C_2H_4	A	F_{A0}	$-F_{A0}X$	$F_{A0}(1-X)$
O_2	B	$\frac{1}{2} F_{A0}$	$-\frac{F_{A0}}{2} X$	$\frac{F_{A0}}{2}(1-X)$
C_2H_4O	C	0	$F_{A0} X$	$F_{A0} X$
Total		$F_{T0} = F_{A0} + \frac{1}{2} F_{A0}$ $F_{T0} = \frac{3}{2} F_{A0}$		$F_T = F_{A0} - F_{A0}X + \frac{F_{A0}}{2} - \frac{F_{A0}}{2} X + F_{A0}X$ $F_T = \frac{3}{2} F_{A0} - \frac{F_{A0}}{2} X$ $F_{A0}\left(\frac{3}{2} - \frac{1}{2}X\right)$

① isobark
① Isothermal

$$C_A = \frac{C_{A0}(1-X)}{1+\varepsilon X} \cancel{\frac{P}{P_0}} \cancel{\frac{T_0}{T}}$$

$\varepsilon = y_{A0}\delta \rightarrow y_{A0} = \frac{1}{1+0.5} = \frac{1}{1.5}$

$\varepsilon = \frac{1}{1.5}\left(1 - \frac{1}{2} - 1\right) = \frac{2}{3}\left(-\frac{1}{2}\right) = -\frac{1}{3}$

$$C_{A0} = \frac{P_{A0}}{RT} = \frac{y_{A0} P}{RT} = \frac{\frac{2}{3} \times 6}{0.08206 \times (260+273)} = 0.0914 \ \frac{mol}{L}$$

$C_A = \frac{0.0914(1-X)}{1-\frac{X}{3}}$; $C_B = \frac{C_{A0}\left(\frac{1}{2} - \frac{1}{2}X\right)}{1+\varepsilon X}$

$C_C = \frac{C_{A0}(0+X)}{1-\frac{X}{3}}$ $C_B = \frac{C_{A0}}{2} \frac{(1-X)}{1-\frac{X}{3}}$

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

$0.15 \rightarrow 0.15 \times \frac{5}{4} \; O_2 = 0.1875$

$\frac{0.15}{4} < \frac{0.21 \times 0.5}{5}$

$0.0375 \qquad 0.0357$

O_2 is the limiting Reactant

3-a

$C_A = C_{A_0}(1-X)$

$C_B = C_{A_0}(0.84 - 0.8X)$

$C_C = 0.8\, C_{A_0} X$

$C_D = 1.2\, C_{A_0} X$

$C_I = 3.76\, C_{A_0}$

$P_T = C_T R T$

$P_T = \sum C_i R T$

3-b

$C_B = \frac{C_{A_0}(0.84 - 0.8X)}{1 + 0.036X}$

$\Theta_B = \frac{y_{B0}}{y_{A0}} = \frac{0.15}{(0.21)(0.85)} = 0.84$

$C_C = C_{A_0}\left(\frac{0 + 0.8X}{1 + 0.036X}\right)$

$C_D = C_{A_0}\left(\frac{0 + 0.8X}{1 + 0.036X}\right)$

$C_I = C_{I_0} = \frac{(0.79)(0.85)(8.2)}{0.082 \times 500}$

$= 0.134 \frac{mol}{L}$

$P_i = C_i R T$

3-b Constan Volume $\quad C_i = C_{A_0}(\Theta_i + \nu_i X)$

Chang Volume $\quad C_i = \frac{C_{A_0}(\Theta_i + \nu_i X)}{1 + \varepsilon X} \frac{P}{P_0} \frac{T_0}{T}$

C_A, C_B, C_C, C_D, C_I

$C_A = C_{A_0} \frac{(1-X)}{1 + \varepsilon X}$ isothermal iso baric $\quad T = T_0 \rightarrow \frac{T}{T_0} = 1 \quad P = P_0 \rightarrow \frac{P}{P_0} = 1$

$\varepsilon = y_{A_0} \delta$

$\varepsilon = \left(\frac{6}{5} + \cancel{\frac{4}{5}} - \cancel{\frac{4}{5}} - 1\right)(0.21 \times 0.85) = 0.035$

$P_{A_0} = y_{A_0} P_T = 0.21 \times 0.85 \times 8.2 = 1.46$ atm

$C_A = 0.036 \frac{(1-X)}{1 + 0.03X} \Big\} \; P_A = C_A R T$

volume.

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$-r_A = k \frac{C_{A0}(1-X)}{1+\varepsilon X} \; \frac{C_{A0}(0.84-0.8X)}{1+\varepsilon X}$

(0905421) Chemical Reaction Engineering I

In-Class Assessment # 9 (Chapter 3)

Partner (1) Name: Sarah.

Partner (2) Name: $= \frac{5000 \times (0.036)^2 (1-X)(0.84-0.8X)}{(1+0.036X)^2}$

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.

$n_{NH_3} = \frac{0.15}{4}$ $\quad n_{O_2} = 0.21 \times \frac{0.85}{5} = 0.0$

$$4NH_3 + 5O_2 \xrightarrow{5} 4NO + 6H_2O$$

~~$4A + 5B \rightarrow 4C$~~ $+ 6D$

$\frac{4}{5}B + A \rightarrow \frac{4}{5}C + \frac{6}{5}D$

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

85% air → 21% O_2, 79% N_2

1. What is the total entering concentration?
2. What is the entering concentration of ammonia?
3. Set up a stoichiometric table with ammonia as your basis of calculation.
   - ✓ a. Express C_i for all species as functions of conversion for a constant-volume batch reactor. Express P_T as a function of X.
   - × b. Express P_i and C_i for all species as functions of conversion for a flow reactor.
4. 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 $L/(mol.min)$.

non elemtly Reaction.

1. $C_{T_0} = \frac{P_T}{RT} = \frac{8.2 \text{ atm}}{0.08206 \frac{\text{atm.L}}{\text{mol.K}} \times (227+273) K} = 0.2 \frac{mol}{L}$

2. $C_{NH_{3_0}} = \frac{0.15 P_T}{RT} = 0.15 \times 0.2 = 0.03 \frac{mol}{L}$

$C_{A0} = C_{O_{2_0}} = 0.85 \times 0.21 \times (0.2) = \frac{0.21 \times 0.85 \times 8.2}{0.08206 \times (227+273)} = 0.036 \frac{mol}{L}$

leving

3.

Species	Symbol	Entring	Chang	
NH_3	~~A~~ B	0.84 N_{A0} ~~N_{A0}~~	~~$-N_{A0}X$~~ $-\frac{4}{5}N_{A0}X$	$(0.84 - \frac{4}{5}X)N_{A0}$
O_2	~~B~~ A	~~1.2~~ N_{A0}	$-N_{A0}X$ ~~$-\frac{5}{4}N_{A0}X$~~	$N_{A0}(1-X)$
NO	C	—	$+\frac{4}{5}N_{A0}X$	$0.8\, N_{A0}X$
H_2O	D	—	$\frac{6}{5}N_{A0}X$	$1.2\, N_{A0}X$
N_2	I	~~4.5~~ N_{A0} 3.76	—	$3.76 N_{A0}$

[illegible]

④ $-r_A = k C_A^1 C_B^1$

$-r_A = k\, C_{A0}(1-X)\, C_{A0}(0.84-0.8X)$

const volume

$= 5000 \times (0.036)^2 (1-X)(0.84-0.8X)$

$\Theta_B = \frac{y_{B0}}{y_{A0}} = \frac{0.21 \times 0.85}{0.15} = 1.2 \quad 1.2^{-1} =$

$\Theta_I = \frac{y_{I0}}{y_{A0}} = \frac{0.79 \times 0.85}{0.15} = 4.5$

School of Engineering
Chemical Engineering Department

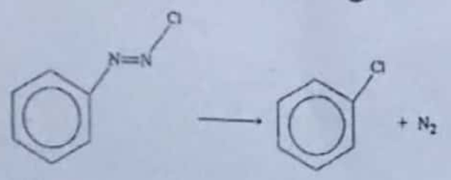
(0905421) Chemical Reaction Engineering I | **In-Class Assessment # 10 (Chapter 3)**

Partner (1) Name: Sarah. **Partner (2) Name:** ______

Identity (1) #: ______ **Identity (2) #:** ______

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:

$\ln K = \ln A - \frac{E}{RT}$



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

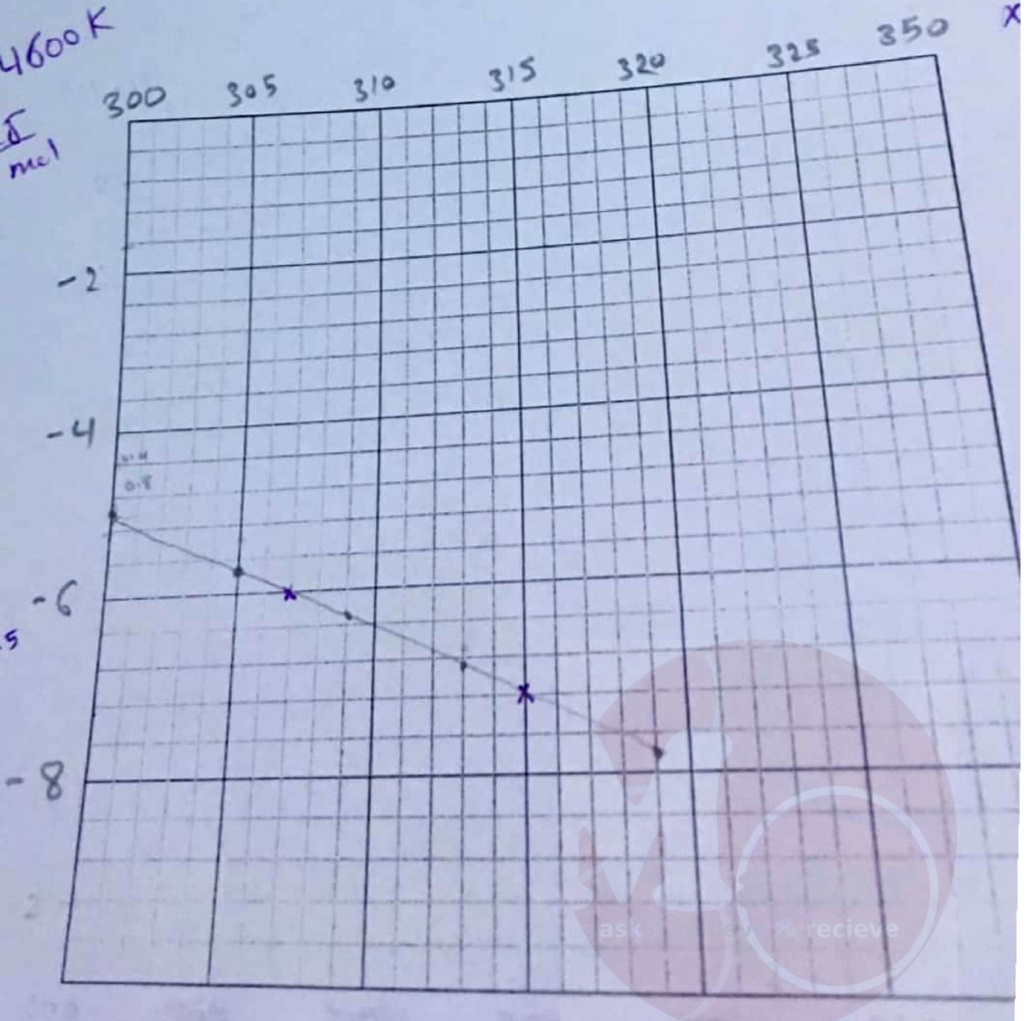
$\ln K$ =	-7.75	-6.88	-6.32	-5.64	-4.94
$\frac{1}{T}$ =	0.00319	0.00313	0.00309	0.00305	0.00300

319×10^{-5}

3.2

slope = −14600 K

$E = 121 \frac{kJ}{mol}$



(307, −6)

(315, −7.2)

$$\text{slope} = \frac{-7.2 - -6}{(315-307)\times10^{-5}} = -15000\,K = \frac{-E}{R}$$

$E = 121 \frac{kJ}{mol}$

(0905421) Chemical Reaction Engineering I

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

Identity (1) #: [illegible] Identity (2) #: ______________________

4.4 Tubular Reactors

The *differential form* of the PFR design equation

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

As an example, consider the reaction

$$A \longrightarrow \text{Products}$$

for which the rate law is

$$-r_A = kC_A^2$$

Gas Phase

For constant-temperature ($T = T_0$) and constant-pressure ($P = P_0$) *gas-phase reactions*, the concentration is expressed as a function of conversion:

$$C_A = \frac{F_A}{v} = \frac{F_A}{v_0(1+\varepsilon X)} = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)} = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}$$

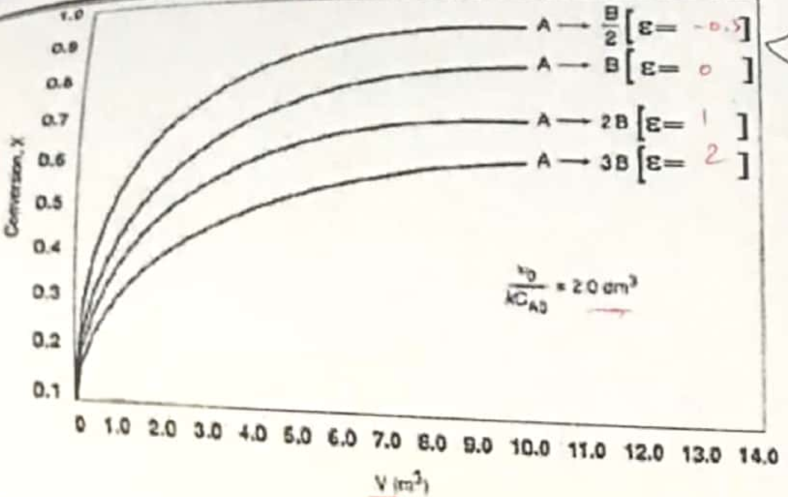
and then combining the PFR mole balance, rate law, and stoichiometry

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

From the integral equations in Appendix A.1, we find that

$$V = \frac{v_0}{kC_{A0}}\left[2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X}\right] \qquad (4\text{-}17)$$

Using Equation (4-17), a plot of conversion along the length (i.e., volume) of the reactor is shown for four different reactions, and values of ε are given in Figure 4-7 for the same value of $[v_0/kC_{A0}]$ to illustrate the effect of volume change with reaction.



Question 1

Find ε in each of the 4 cases shown in Figure 4-7, where the feed consists of pure A.

$y_{A0} = 1$
$\varepsilon = y_{A0}\,\delta$

Figure 4-7 Conversion as a function of distance down the reactor.

We now look at the effect of the change in the number of moles in the gas phase on the relationship between conversion and volume. For constant temperature and pressure, Equation (3-45) becomes

$$v = v_0(1 + \varepsilon X) \tag{3-45}$$

Let's now consider three types of reactions, one in which $\varepsilon = 0$ ($\delta = 0$), one in which $\varepsilon < 0$ ($\delta < 0$), and one in which $\varepsilon > 0$ ($\delta > 0$). When there is no change in the number of moles with reaction, (e.g., $A \rightarrow B$) $\delta = 0$ and $\varepsilon = 0$: then the fluid moves through the reactor at a constant volumetric flow rate ($v = v_0$) as the conversion increases.

When there is a decrease in the number of moles ($\delta < 0$, $\varepsilon < 0$) in the gas phase (e.g., $2A \rightarrow B$), the volumetric gas flow rate decreases as the conversion increases; for example,

$$v = v_0(1 - 0.5X)$$

Consequently, the gas molecules will spend longer in the reactor than they would if the flow rate were constant, $v = v_0$. As a result, this longer residence time would result in a higher conversion than if the flow were constant at v_0.

On the other hand, if there is an increase in the total number of moles ($\delta > 0$, $\varepsilon > 0$) in the gas phase (e.g., $A \rightarrow 2B$), then the volumetric flow rate will increase as the conversion increases; for example,

$$v = v_0(1 + X)$$

$v = v_0(1 + \varepsilon X)$

and the molecules will spend less time in the reactor than they would if the volumetric flow rate were constant. As a result of this smaller residence time in the reactor the conversion will be less than what would result if the volumetric flow rate were constant at v_0.

$\varepsilon \uparrow\ v \uparrow$
at const. volume of React

conversion ↓ ← Residence time ← ↓ $\tau = \frac{V}{v_0 \uparrow}$

Question 2 - After reading the previous 2 pages:

(a) What is the relation between ε and the conversion X? $\varepsilon \uparrow\ X \downarrow$ at the same volume.

(b) In your own words, explain the reason behind this relation.

[illegible] molecules inside React

$\varepsilon \uparrow \Rightarrow v \uparrow$
$\Rightarrow \tau =$ less time is available for molecules to react inside the reactor $\Rightarrow X \downarrow$

(0905421) Chemical Reaction Engineering I **In-Class Assessment # 15 (Chapter 4)**

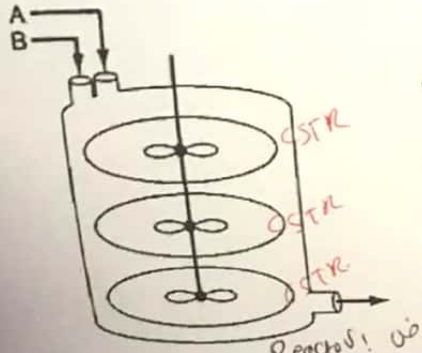
Partner (1) Name: ____________________ **Partner (2) Name:** ____________________

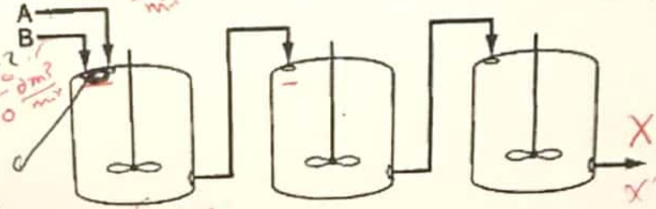
Identity (1) #: ____________________ **Identity (2) #:** ____________________

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 dm³ and the volumetric flow to the first reactor is 10 dm³/min of A and 10 dm³/min of B.

δ ثابت

concentra تتغير عدد المولات ،





$C_{A0} = 2$ $\upsilon_0 = 10 \frac{dm^3}{min}$

$C_{B0} = 2$ $\upsilon_0 = 10 \frac{dm^3}{min}$

200 dm³

$X = 0.488$

X??

C_{A0} الي ندخل Reactor!

$$C_{A_0} = \frac{F_{A0}}{\upsilon_0} = \frac{2 \times 10}{10+10} = \frac{1\,mol}{dm^3}$$ ✓

$$\tau = \frac{V}{\upsilon_0} = \frac{200}{20} = 10\,min$$

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

$C_{A0} = C_{B0} = 2.0$ mol/dm³

k = 0.025 dm³/mol/min

$$-r_A = K C_A C_B = K C_A^{2}$$

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

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

$$\frac{C_{B0}}{C_{A0}} = \frac{2}{2} = 1$$

$$X = 1 - \frac{1}{(1+D_a)^3}$$

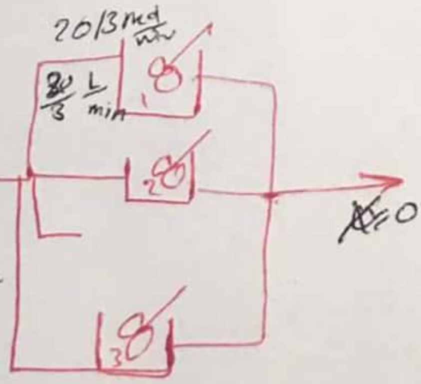
$$D_a = K \tau C_{A0}$$

$$= 0.025 \times 10 \times 1$$

$$= 0.25$$

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

$$\boxed{X = 0.49}$$



$F_{A0} = 2 \times 10 = 20\,\frac{mol}{min}$

$\upsilon_0 = 20\,\frac{L}{min}$

$X = 0.333$

$$V_1 = \frac{F_{A0} X_1}{-r_{A1}}$$

$$200 = \frac{20/3 \quad X_1}{(0.025)(1)^2(1-X)^2} \qquad X = 0.333$$

تتغير concentration

The University of Jordan
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Chemical Engineering Department

(0905421) Chemical Reaction Engineering I	**In-Class Assessment # 13 (Chapter 4)**
Partner (1) Name: ______	**Partner (2) Name:** ______
Identity (1) #: ______	**Identity (2) #:** ______

an elementary

P4-13 Compound A undergoes a reversible isomerization reaction, A ⇄ 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:

PBR

$w_1 = w_2$

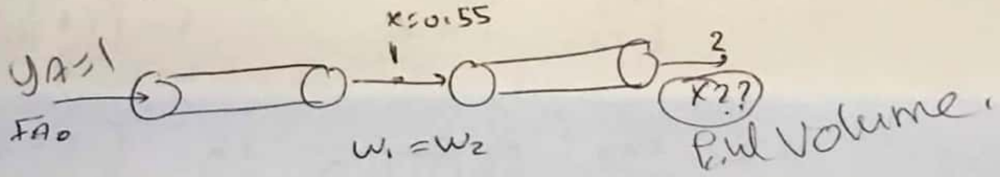
Kc ثابت

(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.*



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

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

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

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

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?

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

$$C_B = C_{A0}X$$

$$\frac{dX}{dW} = \frac{kC_{A0}\left((1-X) - \frac{X}{K_c}\right)}{F_{A0}}$$

$$\int_{x_1 = 0.55}^{x_2} \frac{dx}{(1-x) - \frac{x}{K_c}} = \frac{kC_{A0}}{F_{A0}} \int_0^{W_2} dW = 0.88$$

$W_1 = W_2$

$$\int_0^{0.55} \frac{dx}{(1-x) - \frac{x}{K_c}} = \frac{kC_{A0}W_1}{F_{A0}} = 0.88$$

$$W_1 = \frac{F_{A0}}{kC_{A0}} \frac{1}{1+\frac{1}{K_c}} \ln \frac{1}{1-\left(1+\frac{1}{K_c}\right)x_1}$$

$$= \frac{F_{A0}}{kC_{A0}} \left(\frac{1}{\left(1+\frac{1}{K_c}\right)} \ln \left(\frac{1-\left(1+\frac{1}{K_c}\right)}{1-\left(1+\frac{1}{K_c}\right)}\right.\right.$$

$$x_2 = \left[\frac{1-\left(1-1+\frac{1}{K_c}\right)x_1)?}{1+\frac{1}{K_c}}\right]$$

في الحالة الثانية لما نشيل B كمية Flow rate أقل

نفس weigh of catalest فا بزيد residence time وبالتالي

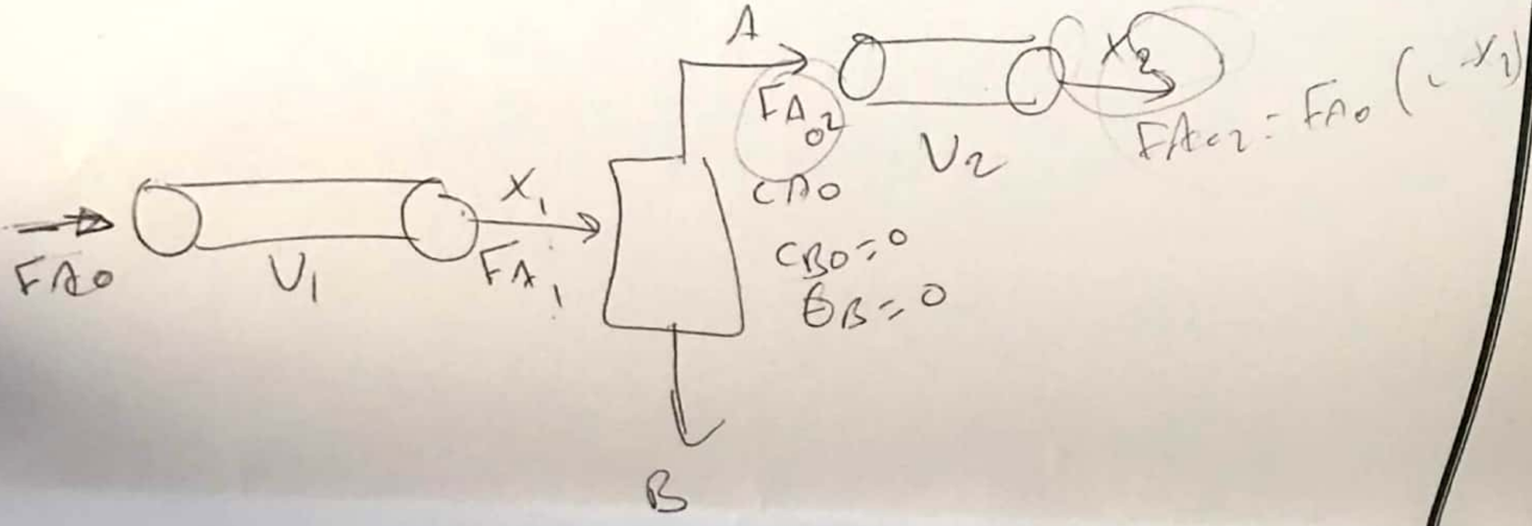
بزيد Conversion.

$x_2' = 0.768$

$$X_{ove\ all} = \frac{F_{A0} - F_{A2}}{F_{A0}}$$

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).

5- Finally, solve the equation you got in (4) and find X_2.



$$F_{A02} = F_{A0}(1-X)$$

$$V_2 = F_{A02}\int_0^{X_2} \frac{dx}{-r_A}$$

$$V_2 = \frac{F_{A0}(1-X_1)}{K\,C_{A0}} \int_0^{X_2} \frac{dx}{(1-x)-\frac{x}{K_{eq}}}$$

$X_{\text{over all}} = 0.895$

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Chemical Engineering Department

(0905421) Chemical Reaction Engineering I **In-Class Assessment # 12 (Chapter 4)**

Name: سميره سليمان فلاح أبو زينة **Identity #:** 0154089

c.o.

Q1: The elementary liquid phase reaction A + B → C is carried out in a CSTR. The initial concentrations of A and B in the entering stream are both 2M, and the specific reaction rate is 0.01 dm^3/(mol.min). Assuming a stoichiometric feed (10 mol A/min) to the reactor: Calculate the reactor volume to achieve 90% conversion. 1c

F_{A0}

Solution: *Follow the algorithm step-by-step:*

0- Write down all given information: C_{A0}, C_{B0}, k, F_{A0}, F_{B0}, v_0, and X.

$C_{A0} = 2M$

$C_{B0} = 2M$

$K = 0.01 \frac{dm3}{mol.min}$

$F_{A0} = 10 \frac{mol}{min}$

$F_{B0} = 10 \frac{mol}{min}$

$v_0 = \frac{10}{2} = 5 \frac{L}{min}$

$X = 0.9$

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

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

3- Do the **stoichiometry (i.e. write the concentration of species appearing in the rate la** Ask yourself again: Is it *liquid or gas phase*? *Constant volume* **terms of conversion).**

The University of Jordan
School of Engineering
Chemical Engineering Department

(0905421) Chemical Reaction Engineering I | **In-Class Assessment # 12 (Chapter 4)**

Name: شفاء عمر السلول

Identity #: 0145594

$v = v_0$

Q1: The elementary liquid phase reaction A + B → C is carried out in a CSTR. The initial concentrations of A and B in the entering stream are both 2M, and the specific reaction rate is 0.01 dm³/(mol.min). Assuming a stoichiometric feed (10 mol A/min) to the reactor: Calculate the reactor volume to achieve 90% conversion.

k

F_A L/min

Solution: *Follow the algorithm step-by-step:*

0- Write down all given information: C_{A0}, C_{B0}, k, F_{A0}, F_{B0}, v_0, and X.

$C_{A_0} = 2M$

$C_{B_0} = 2M$

$k = 0.01 \frac{dm^3}{mol \cdot min}$

$F_{A_0} = 10 \frac{mol\,A}{min}$

$F_{B_0} = 10 \frac{mol\,B}{min}$

$X = 90\%$

$v_0 = 5 \frac{L}{min}$

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

$$V = \frac{F_{A_0} \cdot X}{-r_A}$$

$$F_A - F_{A_0} + r_A \cdot V = 0$$

$$\Rightarrow V = \frac{F_A - F_{A_0}}{-r_A} \Rightarrow \frac{F_{A_0} \cdot X}{-r_A}$$

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

$$-r_A = k_A \cdot C_A C_B$$

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?

$C_A = C_{A_0}(1-X)$

$C_B = C_{A_0}\left(\theta_B - \frac{b}{a} \cdot X\right) \Rightarrow C_{A_0}(1-X)$

$C_C = C_{A_0} \cdot X$

(Liquid phase, constant volume)

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).

$$-r_A = k_A \cdot C_A^2 \cdot (1-X)^2$$

$$V = \frac{F_{A_0} \cdot X}{k \cdot C_{A_0}^2 \cdot (1-X)^2}, \quad V = \frac{V_0 \cdot X}{k \cdot C_{A_0} (1-X)^2}$$

5- Now, solve the equation you got in (4) and find V that will give 90% conversion.

$$V = \frac{V_o \cdot x}{K \cdot C_{A_o} \cdot (1-x)^2} = \frac{5 \times 0.9}{0.01 \times 2 \times (1-0.9)^2} = 22,500 \text{ L}$$

Q2: The following gas phase reaction is first-order in A and zero-order in B;

$$A + B \rightarrow C$$

The reaction is carried out isothermally and isobarically in a **PFR**. The initial concentrations of A and B in the entering stream are both 2M, and the specific reaction rate is 0.01/min. Assuming a stoichiometric feed (10 mol A/min) to the reactor, calculate the reactor volume needed to achieve 90% conversion.

F_{A0}

Solution: *Follow the algorithm step-by-step:*

0- Write down all given information: C_{A0}, C_{B0}, k, F_{A0}, F_{B0}, v_0, and X.

$C_{A0} = 2M$

$C_{B0} = 2M$

$F_{A0} = 10 \frac{mol}{min}$

$X = 0.9$

$k = 0.01 \frac{1}{min}$

$V = V_0$

$V/V_0 = 1$

$v_0 = \frac{F_{A0}}{C_{A0}} = \frac{10}{2} = 5 \frac{L}{min}$

$\frac{T}{T_0} = 1$

$P_0/P = 1$

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

$$F_A\Big|_V - F_A\Big|_{V+\Delta V} + r_A \cdot V = 0 \Rightarrow V = \frac{dF_A}{-r_A}$$

2- Write the **rate law**. Ask yourself: is it elementary or does it follow elementary rate law? If not, find the information that allows you to write the correct rate law.

$$-r_A = K_A \cdot C_A^1 \, C_B^0 \Rightarrow -r_A = K_A \cdot C_A$$

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? Which species is the limiting reactant? If it's gas phase, is there a temperature change? Is there a pressure drop? What is the value of y_{A0}? δ? ε?

$y_{A0} = 0.5$

$\delta = 1 - 1 - 1 = -1$

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

$C_A = C_{A0}(1-x)/(1-0.5x)$

$C_B = C_{A0}(1-x)/(1-0.5x)$

$C_C = \frac{C_{A0} \cdot X}{1-0.5X}$

/gas phase not constant volume.

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).

$$-r_A = K_A \cdot C_{A0} \times \frac{(1-x)}{(1-0.5x)} \quad , \quad V = F_{A0} \int_0^X \frac{dx}{-r_A} \Rightarrow V = F_{A0} \int_0^X \frac{dx}{K_A \cdot C_{A0} \frac{(1-x)}{(1-0.5X)}}$$

$$V = \frac{V_0}{K_A} \cdot \int_0^X \frac{(1-0.5x)\,dx}{(1-x)}$$

V V_0

5- Now, solve the equation you got in (4) and find V that will give 90% conversion. If you are integrating, make sure to correctly define the boundary conditions (i.e. @ V=0, X=0). Useful integrals are available in Appendix A in your textbook. An example of those integrals is shown below. You may need this one to solve your problem!

$$\int_0^x \frac{(1+ex)dx}{1-x} = (1+\varepsilon)\ln\frac{1}{1-x} - \varepsilon x$$

$$V = \frac{V_0}{k} \cdot \int_0^x \frac{(1-0.5x)\,dx}{(1-x)} = (1+\varepsilon) \cdot \ln\left(\frac{1}{1-x}\right) - \varepsilon x$$

$$= \left((1-0.5)\ln\left(\frac{1}{1-0.9}\right) + (0.5 \times 0.9) \right) \times \frac{5}{0.01}$$

$$= 800.6 \text{ L}$$

Differential Method
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 formulas[1]

$$\frac{-3\times 1 + 4\times 0.6 - 0.4}{2\times 10}$$

Initial point:

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

Interior points:

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

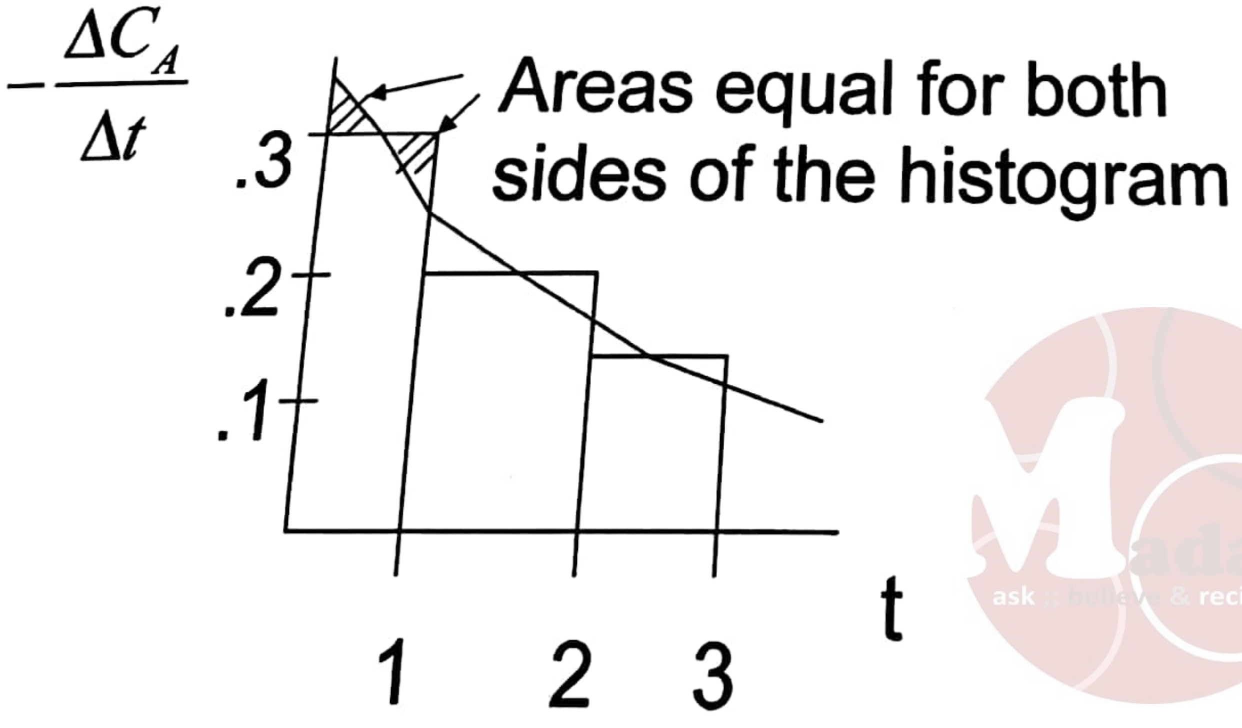
$$\frac{0.4-1}{2\times 10} = -0.03$$

$$\frac{0.3-0.6}{2\times 10} = 0.015$$

Last point:

$$\underline{\left(\frac{dC_A}{dt}\right)_{t_5}} = \frac{1}{2\Delta t}[C_{A3}-4C_{A4}+3C_{A5}]$$

$$\frac{3\times 6.3 - 4\times 0.4 + 0.}{2\times 10}$$



Engineering Department

Chemical Reaction Engineering I

In-Class Assessment # 18 (Chapter 5)

Partner (1) Name: ____________________ **Partner (2) Name:** ____________________

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

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

Numerical

$-\frac{\partial C_A}{\partial t}$	0.05	0.03	0.015	0.005
t (min)	0	10	20	30
C_A(mol/dm^3)	1	0.6	0.4	0.3
$-\frac{\Delta C_A}{\Delta t}$	[illegible]	+0.04	+0.02	+0.01
$-\frac{\partial C_A}{\partial t}$	0.052	0.028	0.015	0.007
ln CA	0	-0.51	-0.921	-1.2
$\ln(-\frac{\partial C_A}{\partial t})$	-2.9	-3.6	-4.2	-4.9

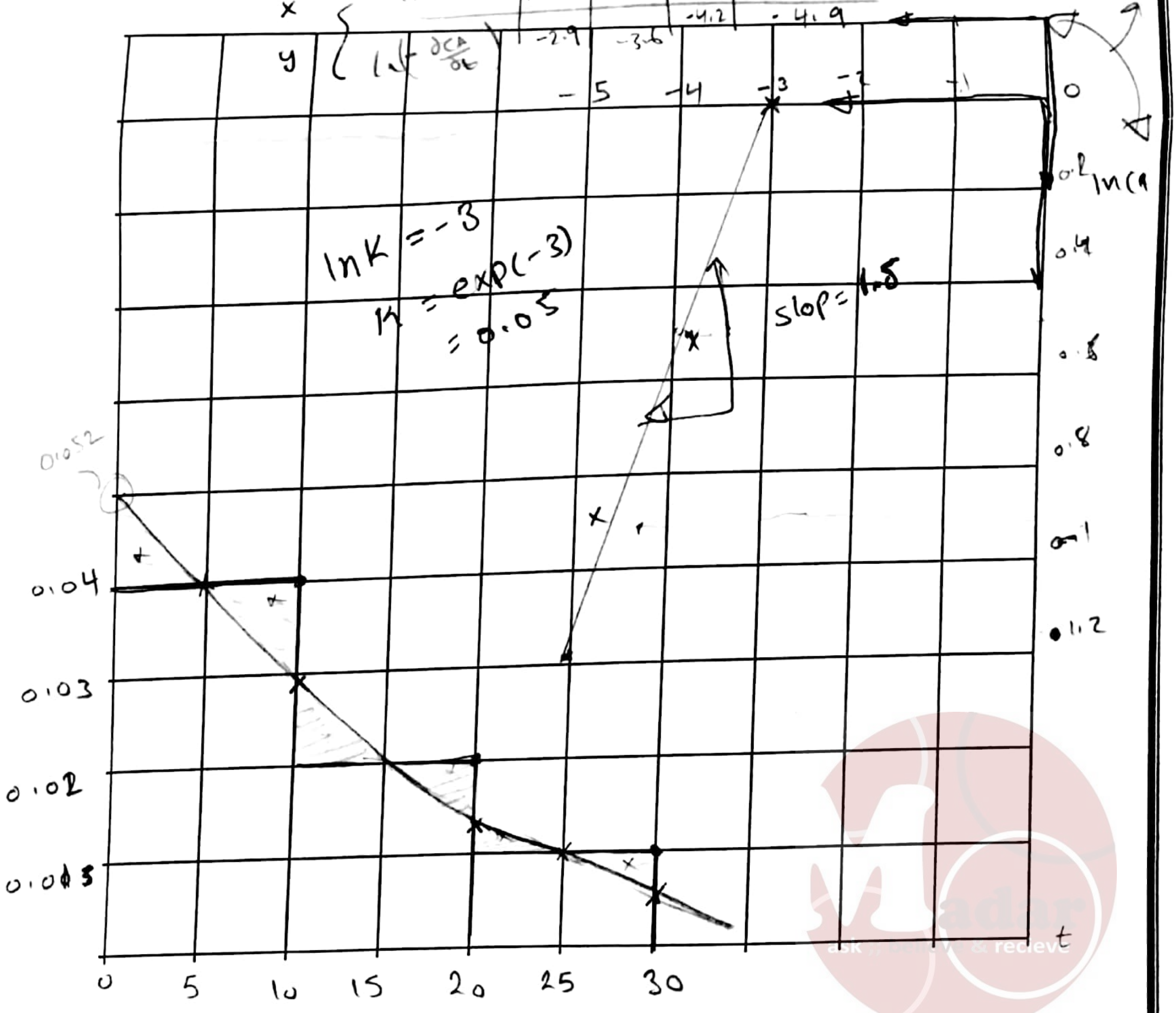
$-\frac{\partial C_A}{\partial t} = k C_A^{\alpha}$

$\ln -\left(\frac{\partial C_A}{\partial t}\right) = \ln k + \alpha \ln C_A$

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

x ln CA

y $\ln(-\frac{\partial C_A}{\partial t})$



$\ln K = -3$

$K = \exp(-3)$

$= 0.05$

slop = 1.5

The oxidation of propene (P) to acrolein (A) was carried out over a Mo-Pr-Bi catalyst [*Ind. Eng. Chem. Res.*, 26, 1419 (1987)].

$$CH_3CH{=}CH_2 + O_2 \rightarrow CH_2{=}CHCHO + H_2O$$

It has been proposed to correlate the data using the power law model for the rate law:

Aclorine → A.

$$r'_{acrolein} = kP_P^{\alpha} P_{O_2}^{\beta}$$

$-r_A' = \frac{F_A}{\Delta W}$ ← product

The reaction was carried out in a differential reactor with 0.5 g of catalyst at 623 K. From the data below, determine the reaction orders with respect to propene (α) and oxygen (β) and the specific reaction rate, ***k***.

F_A (mmol/h)	0.21	0.48	0.09	0.39	0.6	0.14	1.44
P_P (atm)	0.1	0.2	0.05	0.3	0.4	0.05	0.5
P_{O_2}	0.1	0.2	0.05	0.01	0.02	0.4	0.5

intering partial press P, O2 differ

k, α, β P!

where

intering = ~~[illegible]~~

F_A =exiting molar flow rate of acrolein, mmol/h
P_P = entering partial pressure of propene, atm
P_{O_2} = entering partial pressure of oxygen, atm

1, 2, 3, 7

$P_{O_2} = P_P$

$$\ln r_A' = \ln k + \alpha \ln P_P + (\overset{slope}{\beta} - \alpha) \ln P_{O_2}$$

$$\ln r_A' - \ln k - \overset{slope}{} \ln P_{O_2} = \alpha (\ln P_P - \ln P_{O_2})$$

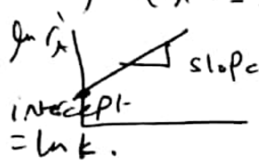
$$\ln \frac{r_A'}{k P_{O_2}} - \text{slope for } P_{O_2} = \alpha \ln \frac{P_P}{P_{O_2}}$$

slope s α

α + β → β ✓

$$r_A' = k P_P^{\alpha} P_{O_2}^{\beta} = k P_P^{\alpha} P_P^{\beta} = k P_P^{\alpha+\beta}$$

$$\ln (r_A') = \ln k + (\alpha + \beta) \ln P_P$$



$$r_A' = k P_P^{\alpha} P_{O_2}^{\beta} \rightarrow \ln r_A' = \ln k + \alpha \ln$$

β ln

The University of Jordan
School of Engineering
Chemical Engineering Department

(0905421) Chemical Reaction Engineering I	**In-Class Assessment # 19 (Chapter 5)**
Partner (1) Name: ____________	**Partner (2) Name:** ____________
Partner (1) ID #: ____________	**Partner (2) ID #:** ____________

$\epsilon = 0$

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.

	100					110.
Run	**1**	**2**	**3**	**4**	**5**	**6**
Initial Concentration, C_{A0} (mol/L)	0.025	0.0133	0.010	0.05	0.075	0.025
Half-life, $t_{1/2}$ (min)	4.1	7.7	9.8	1.96	1.3	2.0

(a) From the data in the table, determine the reaction order and specific reaction rate.
(b) What is the activation energy for this reaction?

$t_{1/2}$

C_{A0}

$\ln t_{1/2} \rightarrow$ y - axis
$\ln C_{A0} \rightarrow$ x - axis

$\rightarrow$ slope = $1-\alpha$

intercept = $\ln \frac{2^{\alpha-1}-1}{k(\alpha-1)}$

$\alpha = 2$ $\Rightarrow \ln \frac{1}{k}$

$k = 10.5 \rightarrow @ 100°C$ مفروض k هيك تطلع

هيك ركة مفروض تطلع $\leftarrow$

✓ Runs $1 \rightarrow 5$.

ر 6 ← بحسبها k جديدة. ✓

$k = @ 110\,°C \rightarrow$ arhinus law

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