

الملف اللي بين إيديكم هو خلاصه ملاحظات وملخصات
جمعتها خلال دراستي الجامعية،

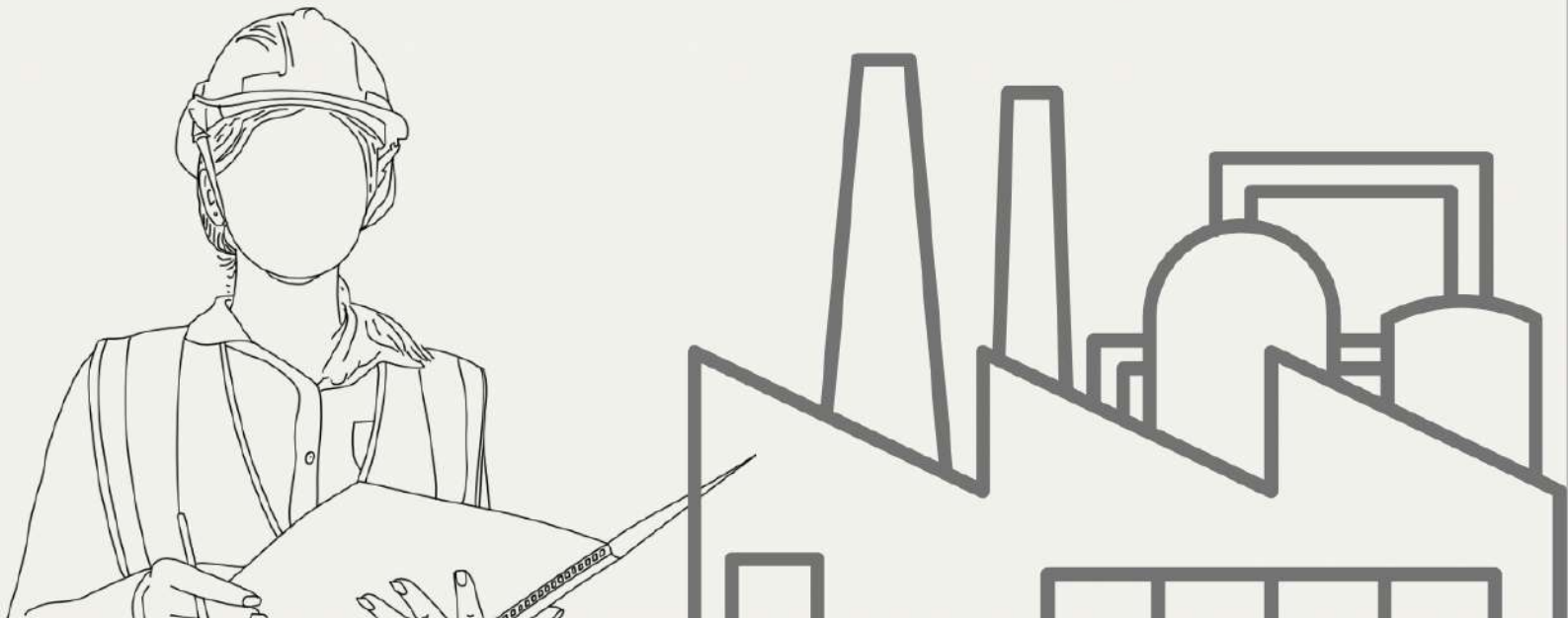
وهو نفس الملف اللي كنت أدرس عليه وأراجع منه وقت
الامتحانات.

حببت أشاركه معكم حتى تستفيدوا منه، ولو بمعلومة صغيرة
أو فكرة بسيطة تساعدكم بالمادة.

ممکن يكون فيه بعض الأخطاء أو النواقص، بس الهدف
الأساسي هو تبادل المعرفة.

من مهندسة كانت طالبة مثلكم،
بحب أحكيلكم: كل تعب بتعيشوه اليوم، رح يكون بكرة سبب
فخرکم بنفسکم.

وما ننسى إنا نحنا كمهندسين كيميائيين، وين ما كنا رح نبدع 🙌
ولا تنسوني من دعوة حلوة 💖



Ch1 Mde Balance

Rate reaction :-



r_A (mol/dm³.s)
per Volume ← homogeneous

$-r_A = 0.2 \rightarrow$ rate disappearance

$r_A = -0.2 \rightarrow$ rate formation

(Heterogeneous) $\rightarrow$ catalytic

$-r_A' \rightarrow$ per mass

$-r_A' = \left(\frac{\text{Kmol}}{\text{Kg.s}} \right) \rightarrow$ catalyst

identity

(product ← reactant) أي مادة تحولت

lost ↓ chemical identity * لازم يكون عيني

+ number + kind 2 تفرع عيني
Configuration

لا يفرع عيني في طريقه :-

de composition $A \rightarrow B + C$

Combination $A + B \rightarrow C$

isomerization $C_2H_5CH=CH_2 \rightarrow$
 $CH_2=C(CH_3)_2$

rate of reaction

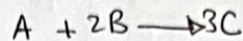
(Batch, CSTR, PTR) reactor بالخز

function (Temp, P, C) هو يكون *

معادلة الجبرك *

General mole balance reaction

example :-



1 rate disappearance of A = $5 \frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}$

$-r_A$? $-r_A \rightarrow$ disappearance

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

2 rate formation of B?

rate disappearance B = $2 \times \text{dissapp}_A$

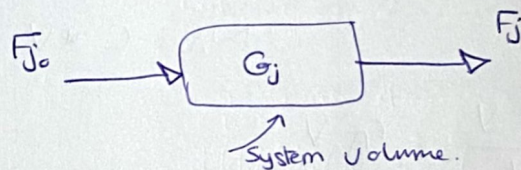
= 2×5
= 10

3 rate formation of C?
rate disappearance = $3 \times \text{rate disappearance}_A$

= $3 \times 5 = 15$

Formation = -15

* General mole balance reaction



$\text{In} + \text{gen} - \text{out} = \text{accum}$

$$F_{j0} - F_j + G_j = \frac{dN_j}{dt}$$

$$F = C \times N_0$$

$$\frac{\text{mole}}{\text{time}} = \frac{\text{mole}}{\text{volume}} \times \frac{\text{volume}}{\text{time}}$$

$N_j =$ no. of mole j at time.

$$N = C \times V$$

$$\text{mole} = \frac{\text{mole}}{\text{volume}} \times \text{volume}$$

$G_j \rightarrow$ Spatially uniform

Constant [T, P, C, catalyst]

$$G_j = r_j \times V$$

non spatially uniform

$$G_j = \sum \Delta G_j = \sum r_j \Delta V_i$$

$$G_j = \int r_j dv$$

مختلطين
①

$$F_{j0} - F_{j1} + \int r_j dV = \frac{dN_j}{dt} \quad \#$$

((Batch, CSTR, PBR, PFR))

Batch reactor

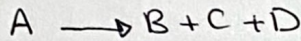
unsteady state

$$F_{A0} = F_A = \text{zero}$$

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

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

example:



(Batch)

- reactor volume
 - concentration
 - rate of reaction
- mole balance $\Rightarrow \sum v_i = 0$

(1)

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

$$N_A = C * V$$

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

(const V (so))

$$V \frac{dC}{dt} = r_A V \rightarrow \frac{dC}{dt} = r_A$$

$$C = \frac{P}{RT}$$

يمكن

(2)

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

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

مرة V و مرة C

$$C \frac{dV}{dt} + V \frac{dC}{dt} = r_A V$$

$$\frac{C}{V} \frac{dV}{dt} + \frac{dC}{dt} = r_A$$

$$\frac{d(CV)}{dt} = r_A V$$

تحت

Continuous stirred tank reactor (CSTR)

liquid أو لولبيات

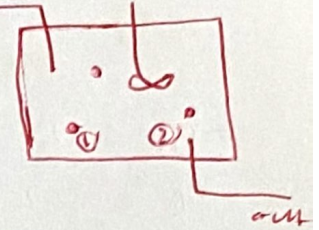
$C, T \rightarrow$ no change time or position

C, T
(constant)

$$V_{in} = V_{out}$$

$$(\text{steady state}) \rightarrow \frac{dN_j}{dt} = 0$$

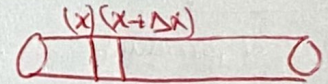
$$V = \frac{F_{j0} - F_j}{-r_j}$$



PFR Tubular reactor

$$\text{Steady state} \rightarrow \frac{dN_j}{dt} = 0$$

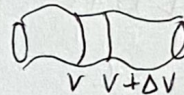
C
Constant



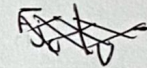
بمساحة مقطع $\rightarrow$ mix

$$F_{j0} \big|_x - F_j \big|_{x+\Delta x} + \int_r r_j dV = 0$$

$$\frac{dF_j}{dV} = r_j$$



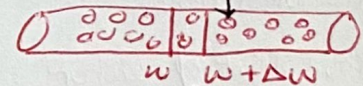
Area مختلف



أقصى

PBR

catalyst reaction



$$\frac{dF}{dW} = r_j'$$

$$V=V$$

تحت

Batch

CSTR

PFR

PBR

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

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

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

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

un st st

well mixed

st st

st st

$$\frac{d(CAV)}{dV} \rightarrow \int dV$$

$v = v_0$
 reduce $\rightarrow 10\%$
 rate = $10 \frac{dm^3}{min}$

$K = 0.23 / min$
 $L_A = 0.1 C_{A0}$

(i) نوع الـ reactor
 (ii) reaction rate
 (iii) معطيات السؤال

(1) Mole balance (PFR)
 reactor نوع

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

r_A reaction rate

$$\frac{dF_A}{dV} = -K C_A$$

هذا قيمة C_A بالـ PFR من بداية
 في البداية

$$\frac{d(C_A \cdot V)}{dV} = -K C_A$$

$$V \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = -K \int_0^V dV$$

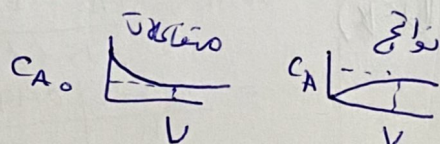
$$\ln C_A \Big|_{C_{A0}}^{C_A} = -\frac{K}{v_0} V$$

$$\ln C_A - \ln C_{A0} = -\frac{K}{v_0} V$$

$$V = \ln \frac{C_A}{C_{A0}} \cdot -\frac{v_0}{K}$$

$$V = \ln \frac{C_{A0} \cdot 0.1}{C_{A0}} \cdot -\frac{10}{0.23}$$

$$V = 100.11 dm^3$$



~~P.1.15~~

$$F_A = F_{A0} - \text{Reacted } (v_0 \cdot X)$$

$$F_A = F_{A0} - F_{A0} X$$

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

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

$$N_A = N_{A0} (1 - X)$$

P.1.15

CSTR $\rightarrow$ Volume
 PFR $\rightarrow$

Consume 99% of A

$$C_A = 0.01 C_{A0}$$

$$\text{molar flow rate} \rightarrow 5 \frac{mol}{h}$$

$$\text{Volumetric flow rate} \rightarrow 10 \frac{dm^3}{h}$$

(1) نوع الـ reactor

(2) rate reaction?

$$-r_A = K = 0.05 \frac{mol}{dm^3 \cdot h}$$

$$\text{initial} \rightarrow F_{A0} = 5 \frac{mol}{h}$$

$$v_0 = 10 \frac{dm^3}{h}$$

$$F_{A0} = C_{A0} \cdot v_0$$

$$5 = C_{A0} \cdot 10 \Rightarrow C_{A0} = 0.5$$

CSTR (1)

معادلة (2)

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

$$(2) -r_A = K$$

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

$$V = \frac{C_{A0} v_0 - C_A v_0}{K} (1 - 0.99)$$

$$V = \frac{10 \cdot 0.5 - 0.01 \cdot 10}{0.05} (1 - 0.99)$$

$$V = 10 \cdot 0.5 \cdot 0.99 = 4.95$$

(2)

① PFR

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

② $r_A = K$

$$\frac{dF_A}{dV} = -K$$

$$F_A \int_{F_{A_0}}^{F_A} dF_A = \int_{V_0}^V -K dV$$

$$F_A - F_{A_0} = -K(V - V_0)$$

$$F_A - F_{A_0} = -K(V - V_0)$$

$$\frac{5 \times 0.99}{0.05} = 99 \text{ dm}^3 = V$$

~~$r_A = K C_A \rightarrow K = 0.0001/s$~~

① CSTR

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

② rate. $r_A = K C_A$

$$V = \frac{F_{A_0} - F_A}{K C_A}$$

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

$$0.5(1-0.99) = 5 \times 10^{-3} \frac{\text{mol}}{\text{dm}^3}$$

~~$$V = \frac{F_{A_0} - F_A}{K C_A}$$~~

~~$$V = \frac{C_{A_0} - C_A}{K C_A}$$~~

~~$$V = \frac{F_{A_0} - F_A}{K C_A}$$~~

~~$$V = \frac{F_{A_0} - F_{A_0}X}{K C_A}$$~~

$$(F_A = F_{A_0} - F_{A_0}X)$$

$$V = \frac{F_{A_0} X}{K C_A}$$

$$= \frac{5 \text{ mol/hr} \times 0.99}{0.0001 \frac{\text{mol}}{\text{dm}^3} \times 3600 \text{ s/hr}}$$

$$V = 2750 \text{ dm}^3$$

① PFR

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

② $r_A = K C_A$

$$\frac{dF_A}{dV} = -K C_A$$

$$\frac{dC_A}{dV} = -K C_A$$

$$V \frac{dC_A}{dV} = -K C_A$$

$$\frac{dC_A}{C_A} = \frac{-K}{V} dV$$

$$\ln(C_A - C_{A_0}) = \frac{-K}{V}(V - V_0)$$

$$\ln \frac{C_A}{C_{A_0}} = \frac{-K}{V} V$$

$$= \frac{-10 \text{ dm}^3/\text{s}}{0.0001} \ln \left(\frac{C_A}{C_{A_0}} \right) (1-x)$$

$$V = 2127.9 \text{ dm}^3$$

③ $-r_A = K C_A^2 \rightarrow K = 3 \frac{\text{dm}^3}{\text{mol} \cdot \text{h}}$

① $V_{\text{CSTR}} = \frac{F_{A_0} - F_A}{-r_A}$

② rate = $-r_A = K C_A^2$

$$V_{\text{CSTR}} = \frac{F_{A_0} - F_A}{K C_A^2} = \frac{F_{A_0} X}{K C_A^2}$$

$$= \frac{5 \text{ mol/hr} \times 0.99}{3 \frac{\text{dm}^3}{\text{mol} \cdot \text{h}} \times (5 \times 10^{-3})^2}$$

$$= 66000 \text{ dm}^3$$

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

$$r_A \rightarrow r_A = K C_A^2$$

$$\frac{dF_A}{dV} = K C_A^2$$

$$\frac{d C_A V}{dV} = K C_A^2$$

$$\frac{d C_A}{C_A^2} = \frac{K}{V} dV$$

$$\left[\frac{C_A^{-1}}{-1} \right]_{C_{A0}}^{C_A} = -\frac{K V}{V}$$

$$\frac{1}{C_A} - \frac{1}{C_{A0}} = -\frac{K V}{V}$$

$$\frac{1}{3} \left[\frac{1}{0.5} - \frac{1}{5 \times 10^{-3}} \right] = V = 660 \text{ dm}^3$$

(D) Batch

$$\begin{aligned} x &= 0.999 \\ V &= 1000 \text{ dm}^3 \\ C_{A0} &= 0.5 \frac{\text{mol}}{\text{dm}^3} \\ t &=? \end{aligned}$$

(1) Batch

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

$$r_A = K$$

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

$$\int_{N_{A0}}^{N_A} dN_A = \int_0^t K V dt$$

$$N_A - N_{A0} = K V t$$

$$\frac{N_{A0} X}{K V} = t$$

$$N_{A0} = C_{A0} V$$

$$\frac{C_{A0} X}{K} = t$$

$$\frac{0.999 \times 0.5}{0.05} = t \Rightarrow 9.994$$

(2) Batch

$$\text{rate} = K C_A$$

$$\frac{d C_A V}{dt} = r_A V$$

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

$$\frac{d C_A V}{dt} = -K C_A V$$

$$\frac{dN_A}{dt} = -K C_A V$$

$$(6988 \text{ s})$$

$$\int_{N_{A0}}^{N_A} dN_A = -K C_A V dt$$

$$N_{A0} - N_A = -K C_A V t$$

$$\frac{N_{A0} X}{K C_A V} = t$$

$$N_{A0} = C_{A0} V$$

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

$$t = \frac{0.999}{0.001 \times (1-0.999)}$$

$$t = 999000 \text{ s}$$

$$(3) \frac{dN_A}{dt} = r_A V$$

$$r_A = K C_A^2$$

$$\frac{d C_A V}{dt} = -K C_A^2 V$$

$$\frac{d C_A}{C_A^2} = -K dt$$

$$\frac{1}{C_{A0}} - \frac{1}{C_A} = -K t$$

$$t = \frac{1}{3} \left(\frac{1}{0.5} - \frac{1}{0.5(1-0.999)} \right)$$

$$= 666 \text{ h}$$

P. 1-12



gas phase.

$$\begin{cases} V_0 = 20 \text{ dm}^3 \\ \text{batch reactor} \end{cases}$$

② $N_{A0} = 20$ well mix

$$\begin{cases} -r_A = K C_A \rightarrow K = 0.865/\text{min} \\ t = ? \quad N_A = 0.2 \text{ mol} \text{ reduce} \end{cases}$$

③ $-r_A = K C_A^2 \rightarrow K = 2 \frac{\text{dm}^3}{\text{mol min}}$
 $t = ? \quad N_A = 19 \text{ mol}$

④ Batch

$$\frac{dN_A}{dt} = r_A V \quad (N_{A0} X)$$

rate $\frac{dN_A}{dt} = -K C_A V$

$$\frac{dC_A V}{dt} = -K C_A V$$

$$\int_{C_0}^C \frac{dC_A}{C_A} = -K dt$$

$$\ln\left(\frac{C_{A0}}{C_A}\right) = -K t \quad C_A = \frac{N}{V}$$

$$\frac{1 \text{ min}}{-0.865} \mid \ln\left(\frac{0.2}{20}\right) = t$$

$$t = 5.3 \text{ min}$$

⑤ Batch

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

rate $-r_A = K C_A^2$

$$\frac{dN_A}{dt} = -K C_A^2 V$$

$$\frac{dC_A}{dt} = -K C_A^2$$

$$\frac{1}{K} \left[\frac{1}{C_{A0}} - \frac{1}{C_A} \right] = t$$

$$N_A = N_{A0} - N_{A0} X$$

$$= 20 - 19 = 1 \text{ mol}$$

$$t = -\frac{20}{2} \left[\frac{1}{20} - \frac{1}{1} \right] = 9.5 \text{ min}$$

example



time = ?

$$N_{A0} \downarrow 10$$

batch, $-r_A = K C_A$
 $K = 0.046 \text{ min}^{-1}$

① batch

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

rate $= -r_A = K C_A$

$$\frac{dC_A}{dt} = -K C_A$$

$$\frac{dC_A}{C_A} = -K dt$$

$$\ln\left(\frac{C_{A0}}{C_A}\right) = K t$$

$$\frac{C_{A0}}{C_A} = \frac{N_{A0}}{N_A}$$

$$t = -\frac{1}{K} \ln \frac{0.1 N_{A0}}{N_{A0}}$$

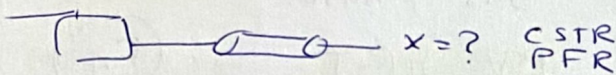
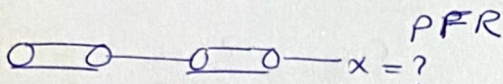
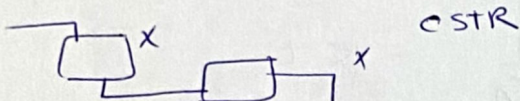
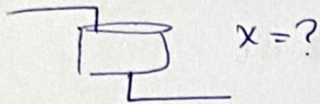
$$t = 50.05 \text{ min}$$

Ch2 Conversion of Reactor sizing.

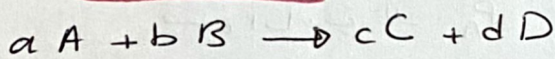
① Size a reactor → CSTR
→ PFR

② Conversion ??

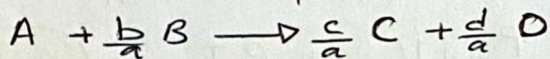
③ Reactors in series → CSTR
→ PFR
CSTR PFR



2.1 Conversion ??



أو a مولات A و b مولات B ينتجان c مولات C و d مولات D



10 mol Feed A → mol C ??

2 mol A
المولات

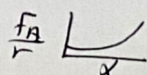
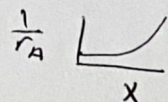
المولات المولدة من A

$$X = \frac{\text{mole reacted } A}{\text{mole Feed } A}$$

$$X_{\max} = X_{\text{equilibrium}}$$

$$\frac{X}{r_A}$$

أو $\frac{1}{r_A}$



(Time $\uparrow$ X $\uparrow$)

2.2 Batch reactor :-

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

$$N_A = N_{A0} - N_{A0} X$$

$$N_{A0} \frac{dX}{dt} = -r_A V$$

$$\frac{dCA}{dt} = -r_A$$

CSTR reactor

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

PFR reactor

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

PBR reactor

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

$$F_{A0} = \frac{C_{A0} V}{\tau}$$

أو

$$P_0 V = nRT_0$$

$$\frac{n}{V} = C_{A0}$$

$$\frac{P_{\text{total}} \cdot y_{A0}}{RT} = C_A$$

$$X_{\max} = ? = 1$$

$$-r_A = 0$$

$$\frac{1}{r_A} \rightarrow \infty$$

أو

$$A \longrightarrow B$$

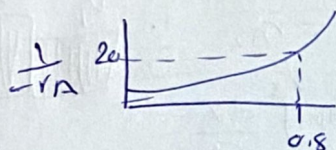
Conversion
 $X = 80\%$

$$F_{Ac} = 0.4 \frac{\text{md}}{\text{s}}$$

CSTR

$$V = \frac{F_A \cdot X}{r_A} = \frac{0.4 \times 0.8 \times 20}{1} = 6.4$$

* كَوَيْل الوَصَدَات بِكُونِ sec , hr

 V_{PFR}

$$F_A \circ \frac{dX}{dV} = -r_A$$

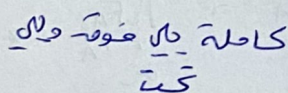
$$F_A dx = -r_A dV$$

$$F_{A_0} dx = -r_A V$$

$$F_{Ac} \int_0^{0.8} \frac{dx}{-r_A}$$

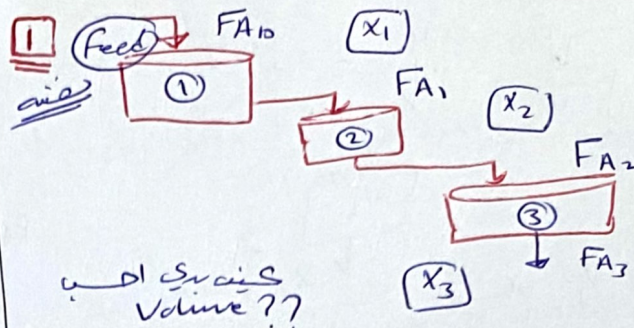
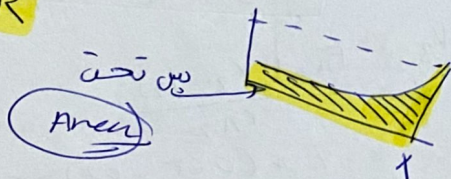
* نیند میرکال *

CSTR $\rightarrow$ Volume $\frac{F_A}{r_A}$



Aven

PFR



$$V_1 = \frac{F_{A_0} X_1}{-r_A} \Big|_{x_1}$$

$$V_2 = ?$$

$$\text{In} - \text{out} + \text{gen} = \cancel{\text{acc}} \circ$$

$$V_2 = \frac{F_{A1} - F_{A2}}{-r_A |_{x_2}}$$

$$V_3 = \frac{FA_2 - FA_3}{-r_A \parallel x_3} \rightarrow \text{tabel}$$

$$\bar{F}_{A_1} = F_{A_0} - F_{A_0} X_1$$

$$F_{A_2} = F_{A_1} - F_{A_0} X_2$$

$$F_{A_3} = F_{A_0} - F_{A_0} X_3$$

$$* V_2 = \frac{F_{A_0} (x_2 - x_1)}{-r_{A_1} x_2}$$

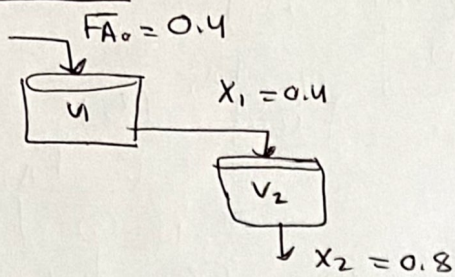
$$* V_3 = \frac{F_{A_0} (x_3 - x_2)}{-r_{A_1} x_3}$$

$$V_{PFR} = F_{A_0} \int \frac{dx}{-r_A}$$

$$V_{CSTR} = \frac{F_{A0} (X_2 - X_1)}{-r_A|_{X_2}}$$

x کل خارجہ عدد CSTR $\leftarrow V \downarrow$

example



$$\therefore V = V_{\text{total}}$$

$$V_{\text{total}} = V_1 + V_2$$

$$V_1 = \frac{F_{A0} X_1}{-r_{A1} \big|_{X_1}} \rightarrow \text{table}$$

$$= (0.4 \times 0.4) \times 5.13$$

$$V_1 = 0.82 \text{ m}^3$$

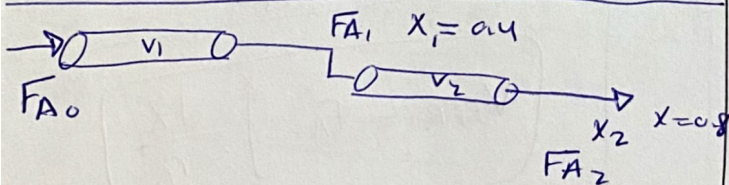
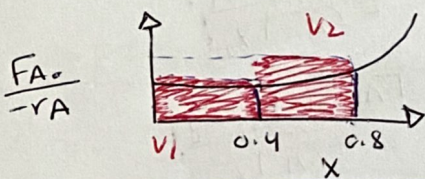
$$V_2 = \frac{F_{A0} (X_2 - X_1)}{-r_{A2} \big|_{X_2}} = 8 \times (0.8 - 0.4)$$

$$V_2 = 3.2 \text{ m}^3$$

$$V_{\text{total}} = V_1 + V_2 = 0.82 + 3.2 = 4.02$$

Series V_1, V_2, V_3 (**) (smiley face)

Conversion X



$$V = V_1 + V_2$$

PFR

$$V_1 = F_{A0} \int_0^{0.4} \frac{dX}{-r_A} = 0.551 \text{ m}^3$$

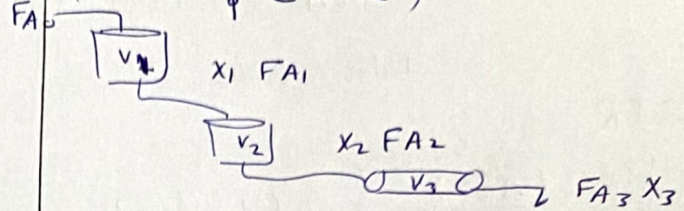
$$V_2 = F_{A0} \int_{0.4}^{0.8} \frac{dX}{-r_A} = 4.614 \text{ m}^3$$

تقسيم القيمة
Series

$$2.165 \text{ m}^3$$



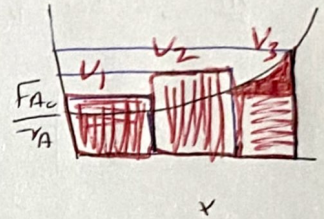
(PFR & CSTR)



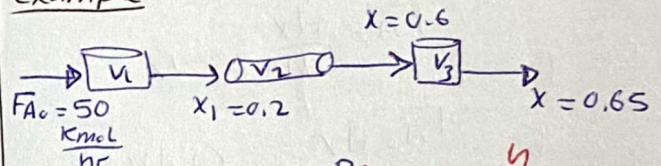
$$V_1 = \frac{F_{A0} X_1}{-r_{A1}}$$

$$V_2 = \frac{F_{A0} X_2}{-r_{A2}}$$

$$V_3 = F_{A0} \int_{X_2}^{X_3} \frac{dX}{-r_A}$$



example



X	0.0	0.2	0.4	0.6	0.8
-rA	34	53	59	38	25

$$\frac{F_{A0}}{-r_A} \bigg|_{X=0.2} = 1.28 \quad \frac{F_{A0}}{-r_A} \bigg|_{X=0.6} = 0.94 \quad \frac{F_{A0}}{-r_A} \bigg|_{X=0.65} = 0.85 \quad \frac{F_{A0}}{-r_A} \bigg|_{X=0.65} = 1.32 \quad \frac{F_{A0}}{-r_A} \bigg|_{X=0.65} = 2.0$$

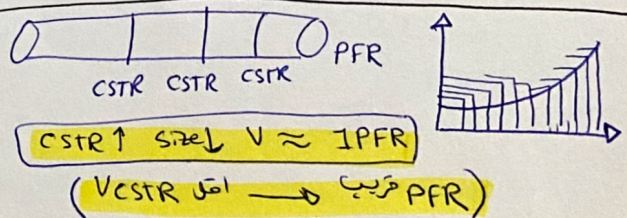
$$V_{1 \text{ CSTR}} = \frac{F_{A0} X}{-r_A} = 0.94 \times 0.2 = 0.188 \text{ m}^3$$

$$V_2 \text{ PFR} = F_{A0} \int_{X_1}^{X_2} \frac{dX}{-r_A} = \int_{0.2}^{0.6} \frac{F_{A0}}{-r_A} dX$$

تقسيم القيمة (Series)

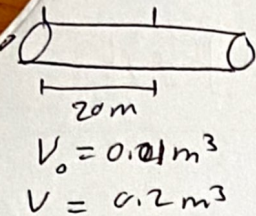
$$\frac{(0.6 - 0.2)}{2 \times 3} [0.94 + 4 \times 0.85 + 1.32]$$

$$V_3 = \frac{F_{A0} (X_2 - X_1)}{-r_A} = 2 \times (0.65 - 0.6) = 0.1 \text{ m}^3$$



CSTR $\uparrow$ size $\downarrow$ $V \approx 1 \text{ PFR}$

(VCSTR $\rightarrow$ قريب PFR)



$$\tau = \frac{V}{V_0} = \frac{0.2}{0.01} = 20 \text{ s}$$

* **time**
 Feed $\rightarrow$ reactor
 Space time

$$SV = \frac{V_0}{V} = \frac{1}{\tau}$$

Space velocity

liquid
 $LHSV = \frac{V_0}{V} \Big|_L$

gas
 $GHSV = \frac{V_0}{V} \Big|_{STP}$

P2.7

X	0	0.2	0.4	0.45	0.5	0.6	0.8	0.9
-r _A	1	1.67	5	5	5	5	1.25	0.9

mol / dm³ min
 $F_{A0} = 300 \text{ mol/min}$
 الوصل

(A) $V_{CSTR} = V_{PFR}$ } $x = 0.4$?

$$[1] V_{CSTR} = \frac{F_{A0} X}{-r_A|_X}$$

$$V_{CSTR} = \frac{300 \times 0.4}{5} = 24 \text{ dm}^3$$

$$[2] V_{PFR} = F_{A0} \int_0^{x_1} \frac{dx}{-r_A}$$

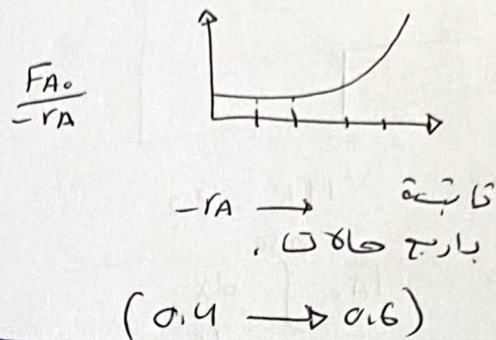
$$= 300 \int_0^{0.4} \frac{dx}{-r_A}$$

(بندریکال) - جیو مع فک الورقه

$$= 300 \times \frac{0.4 - 0}{2 \times 3} \left[\frac{1}{1} + 4 \times \frac{1}{1.65} + \frac{1}{5} \right]$$

$$= 72 \text{ dm}^3$$

$V_{PFR} = V_{CSTR}$
 (B) $V_{CSTR} = \frac{F_{A0} X}{-r_A}$
 $V_{PFR} = F_{A0} \int_0^X \frac{dx}{-r_A}$



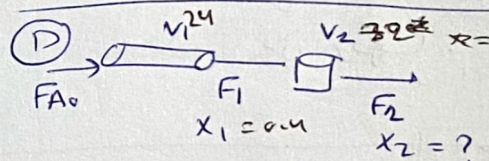
(C) CSTR
 $V = 105 \text{ dm}^3 \Rightarrow X_{max}$

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

$$105 \text{ dm} = \frac{300 \times X}{-r_A}$$

$$\frac{105}{300} = \frac{X}{-r_A} \Rightarrow ??$$

(try and error) خد

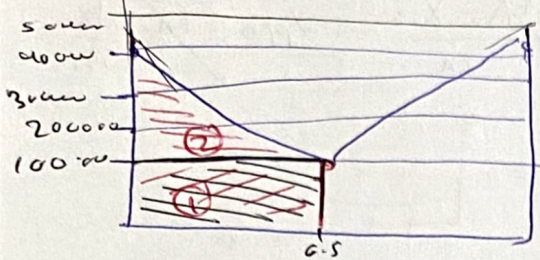
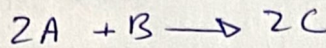


$$V_1 = \frac{F_{A0}(X_2 - X_1)}{-r_A}$$

$$24 = \frac{300 (X_2 - 0.4)}{-r_A}$$

خارجی دین

example P.29



$X = 0.50$

$V_{PFR} = ??$

$$V_{PFR} = F_{A0} \int_0^{0.50} \frac{dX}{-r_A}$$

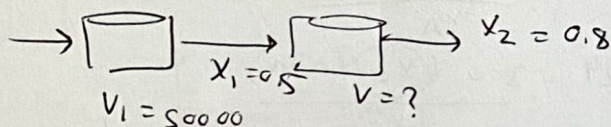
$V_{PFR} = \text{Area} = (\text{المربع} * \text{طول}) + (\frac{1}{2} * 19 * 8)$

$$\int_{\text{curve}} = 0.5 * 100000 + \frac{1}{2} * 0.5 * 40000 = 150000 \text{ m}^3$$

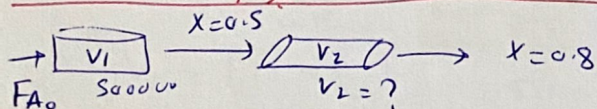
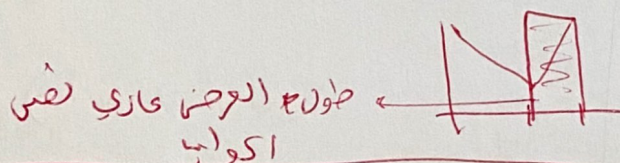
$V_{CSTR} = \text{المربع} * \text{طول}$
 $0.5 * 100000$

حاصلات يال قفا curve
خلص بي بي المنطقة
بي مرقع . سواي قووة
ارتك

$X = 0.80$ بي



$$V_2 = \frac{F_{A0} (X_2 - X_1)}{-r_A|_{X_2}} = \frac{500000 * (0.8 - 0.5)}{-r_A|_{X_2}} = 15000 \text{ m}^3$$



$$V_2 \text{ PFR} = F_{A0} \int_{0.5}^{0.8} \frac{dX}{-r_A} = \int_{0.5}^{0.8} \frac{F_{A0}}{-r_A} dX$$

بي مرقع . اذا اتيه بصل Area تحت المنحنى

$\nabla = \text{Area}$ بار

قوى

$T = 500 \text{ K}$

$P = 101.3 \text{ kPa}$

$y_A = 0.333$

$y_B = 0.667$

(a) $V_{PFR} \rightarrow X = 30\%$
 $V = 2 \frac{\text{m}^3}{\text{min}}$

$V_{PFR} = F_{A0} \int_0^{0.3} \frac{dX}{-r_A}$ بي مرقع

$F_{A0} = ?$

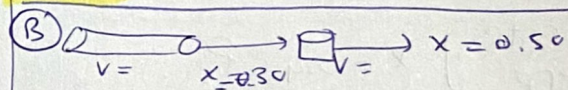
$F_{A0} = C_{A0} * V$
gas

$PV = nRT$

$P = \left(\frac{n}{V} \right) RT$

$(P_{tot} * y_A) = C_{A0} * R * T$

$F_{A0} * \left(\frac{X}{2 * 3} \right) [F_{A0} + 4 F_{A1} + F_{A2}]$



$$V = \frac{F_{A0} (X_2 - X_1)}{-r_A|_{X_2}} = \frac{2.074 * (0.5 - 0.3)}{-0.005}$$

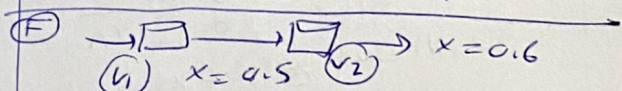
360.5 m^3

(c) $X = 0.60$
 $V_{PFR} = F_{A0} \int_0^{0.60} \frac{dX}{-r_A}$ بي مرقع

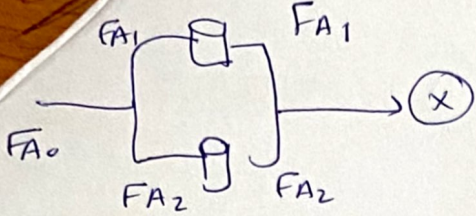
(d) $V_{CSTR} \rightarrow X = 0.50$

$$V = \frac{F_{A0} X}{-r_A} = 2.07 * 0.159$$

اذا كانت
بي مرقع انتر بولي



$$V_{CSTR} = \frac{F_{A0} (X_2 - X_1)}{-r_A|_{X_2 = 0.6}}$$



$$X = \frac{FA_1 X_1 + FA_2 X_2}{FA_1 + FA_2}$$

$$FA_1 = 2FA_2$$

W = Area under the curve * X

Weight

$$FA_0 \int_0^X \frac{dx}{-r_A} = W$$

PFR

(1) given under the curve

سؤال

$X_A = 0.3$

$\frac{1}{\tau} = 0.1 \text{ min}^{-1}$] CSTR

فكر

$\frac{1}{\tau} = 0.2 \text{ min}^{-1}$] PFR

$X_{PFR} = ?$

$-r_A = K$ given

$$VPFR = FA_0 \int_0^X \frac{dx}{-r_A}$$

$$= FA_0 \int_0^X \frac{dx}{K}$$

? $VPFR = FA_0 \frac{X}{K}$?

$$X = \frac{V * K}{CA_0 * \tau}$$

τ

$$X = \tau \frac{K}{CA_0}$$

$$V_{CSTR} = \frac{FA_0 X}{-r_A} = \frac{FA_0 X}{K}$$

$$V = \frac{V_0 * CA_0 X}{K}$$

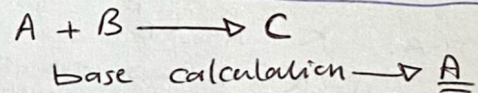
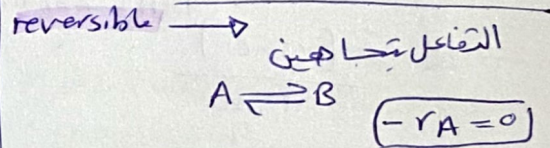
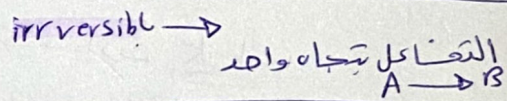
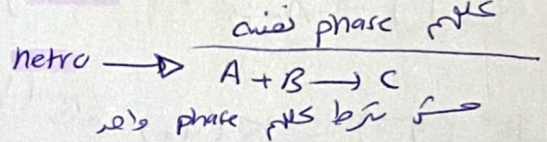
$$\frac{K}{CA_0} = \left(\frac{V_0}{V} \right) * X_{CSTR}$$

$$\frac{K}{CA_0} = \frac{1}{\tau} * X = 0.03$$

PFR

$$PFR^X = \left(\frac{1}{\tau} \right) \left(\frac{K}{CA_0} \right)$$

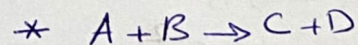
ch3 Basic definitions:-



$$-r_A = f(X, T)$$

$$-r_A = K \frac{CA}{CA_0(1-X)}$$

$\Rightarrow$ isothermal K constant



$$K_A = K_B = K_C = K_D = K$$

كل تفاعل K واحد

$$K(T) = A e^{-E_a/RT}$$

Frequency, pre exponential

$$\frac{1}{\text{Time}} = Hz$$

$E_a \rightarrow$ activation J/mol

$R \rightarrow$ gas const. 8.31 J/molK

$$T \rightarrow K$$

$$-r_A = K C_A$$

$$300 = T \quad \text{اصطفاي}$$

$$K = K$$

$$350 = T \quad \text{مع } K$$

طوب سواغل - !

$$K(T_0) = A e^{-E_a/RT_0}$$

$$K(T) = A e^{-E_a/RT} \quad \text{قسمة}$$

$$K(T) = K(T_0) e^{\frac{E_a}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right)}$$

unit K كيف اوف

$$K = \frac{[\text{conc}]}{\text{Time}} \quad 1-n \rightarrow \text{order}$$

$$-r_A = K C_A^\alpha C_B^\beta$$

$n = \alpha + \beta \rightarrow$ order reaction

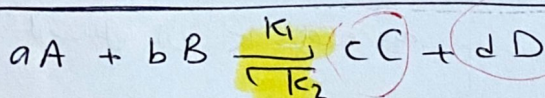


$$-r_A = K C_A^1 C_B^1$$

...

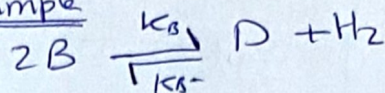


$$-r_A = K C_A^2$$



$$K_c = \frac{(C_c)^c (C_d)^d}{(C_A)^a (C_B)^b} \quad \frac{D}{R}$$

Example

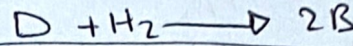


K_B



$$-r_B = K_B C_B^2$$

$-K_B$



$$r_B = K_B C_D C_{H_2}$$

$$K_c = \frac{K_B}{K_B}$$

net $\rightarrow$ العكسي + العكسي

$$r = -r_B + r_B$$

$$r = -K_B C_B^2 + K_B C_D C_{H_2}$$

* $-r_A = g(x)$ بين اطلع علاقة

	Initial	Change	Remaining
A	N_{A0}	$-NA_0X$	$N_{A0} - NA_0X$
B	N_{B0}	$-\frac{b}{a} NA_0X$	$N_{B0} - \frac{b}{a} NA_0X = N_B$
C	N_{C0}	$+\frac{c}{a} NA_0X$	$N_{C0} + \frac{c}{a} NA_0X = N_C$
D	N_{D0}	$+\frac{d}{a} NA_0X$	$N_{D0} + \frac{d}{a} NA_0X = N_D$
I	N_{I0}	-	N_I

$N_T = N_{T0} + \text{change} = N_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \right) NA_0X$

$$A/B = NA_0 \theta_B - \frac{b}{a} X NA_0$$

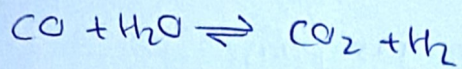
$$\theta_B = \frac{N_{B0}}{NA_0} \quad \theta_D = \frac{N_{D0}}{NA_0}$$

$$\theta_C = \frac{N_{C0}}{NA_0} \quad \theta_A = \theta_B - \theta_C = \theta_D$$

$$C_A = \frac{NA_0}{V}$$

$$C_B = \frac{N_B}{V} = \frac{NA_0 \theta_B - \frac{b}{a} X NA_0}{V_0}$$

$$\theta = \frac{N_i}{N_{A0}} = \frac{C_i}{C_{A0}} = \frac{y_i}{y_{A0}}$$



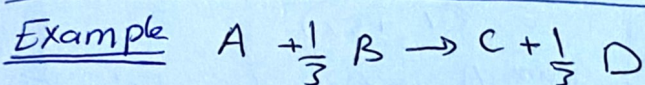
- constant Volume ① liquid
 ② T, P const
 ③ mol out = mol in

$$\delta = 0 \Rightarrow V = V_0$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-x)}{V_0}$$

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

$$C_B = C_{B0}(\theta_B - \frac{b}{a}x)$$



$$\text{mol out} = \text{mol in}$$

$$\frac{1}{3} + 1 = \frac{1}{3} + \frac{1}{3}$$

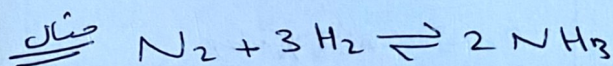
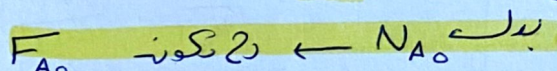
$$V = V_0$$

A	N_{A0}	$N_{A0}x$	$N_{A0}(1-x)$
B	$N_{A0}\theta_B$	$N_{A0}\frac{x}{3}$	$N_{A0}(\theta_B - \frac{1}{3})$
C	$N_{A0}\theta_C$	$N_{A0}\frac{x}{3}$	$N_{A0}(\theta_C + x)$
D	$N_{A0}\theta_D$	$N_{A0}\frac{x}{3}$	$N_{A0}(\theta_D + \frac{x}{3})$

Flow system $\Rightarrow F_{i0}$

Batch No

CSTR
PFR
iso Batch



$$4 \neq 2 \Rightarrow V \neq V_0$$

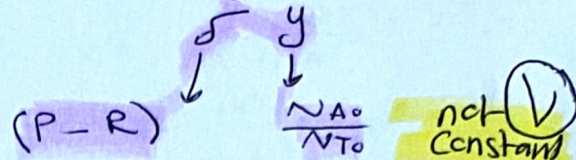
$$PV = Z N_T RT$$

①

Volume ratio

$$V = \frac{t}{t_0} \frac{N_T}{N_{T0}} \cdot \frac{T}{T_0} \cdot \frac{P_0}{P} \cdot V_0$$

$$(1 + \epsilon x)$$



$$V = V_0 \frac{P_0}{P} \frac{Z}{Z_0} \frac{T}{T_0} (1 + \epsilon x)$$

$$C_A = \frac{F_{A0} N_{A0} (1-x)}{V_0 \frac{P_0}{P} \frac{Z}{Z_0} \frac{T}{T_0} (1 + \epsilon x)}$$

$$C = \frac{P}{RT}$$

$$PV = nRT$$

$$P = \frac{n}{V} RTZ$$

$$C = \frac{P}{ZRT}$$

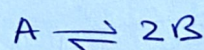
$$C = \frac{F}{V}$$

$$C_{T0} = \frac{F_{T0}}{V_0}$$

* Isothermal $\rightarrow \frac{T}{T_0} = 1$

* neglect P $\rightarrow \frac{P_0}{P} = 1$

Example



gas phase { reversible
 $V \neq V_0$

constant T / Feed pure

$$T = 340K / P = 202.6 \text{ kPa}$$

$$K_c = 0.1$$

①

$$x = ?$$

const

iso

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

reversible $\rightarrow r_A = 0$

$$0 = \left[C_A - \frac{C_B^2}{K_c} \right]$$

$$C_A = \frac{C_B^2}{K_c}$$

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

$$C_B = \frac{N_{A0}(\theta_B + 2x)}{V_0}$$

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

⑧

$$\theta_B = \frac{C_{B0}}{C_{A0}} = 0$$

$$C_B = 2C_{A0}X$$

$$K_c = \frac{(2C_{A0}X)^2}{C_{A0}(1-X)}$$

$$0.1 = \frac{2X C_{A0}}{(1-X)} \rightarrow X$$

$$C_{A0} = \frac{P_A P}{RT}$$

⑥ Flow reactor:-

$$-r_A = K (C_A - \frac{C_B^2}{K_c}) = 0$$

$$K_c = \frac{C_B^2}{C_A}$$

$$C_B = \frac{F_B}{V} = \frac{F_{A0}(\theta_B + 2X)}{V_0 \frac{P}{P_0} \frac{T_0}{T} \frac{Z_0}{Z} (1+\epsilon X)}$$

$$C_B = \frac{F_{A0}(2X)}{V_0(1+\epsilon X)} = \frac{C_{A0}(2X)}{(1+\epsilon X)}$$

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

$$K_c = \left(\frac{C_{A0}(2X)}{(1+\epsilon X)} \right)^2 \left(\frac{C_{A0}(1-X)}{(1+\epsilon X)} \right)^{-1} \quad \Sigma = \sum y$$

P. 316 Liquid $A+B \rightleftharpoons C$

$$C_{A0} = C_{B0} = 2, K_c = 10$$

$$-r_A = (C_A C_B K + \frac{C_C}{K_c})$$

$$-r_A = K (C_A C_B + \frac{C_C}{K_c}) = 0$$

$$K_c = \frac{C_C}{C_A C_B}$$

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

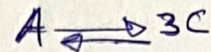
$$C_B = \frac{F_{A0}X}{V_0} = C_{A0}X$$

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

$$C_B = \frac{F_{A0}X}{V_0} = C_{A0}X$$

$$K_c = \frac{C_{A0}X}{C_{A0}^2(1-X)^2} \rightarrow X$$

⑦ gas phase



gas phase

Pure A $T = 400K$

$\Delta P = 0$ $K_c = 25$

$$-r_A = K \left[C_A + \frac{C_C^3}{K_c} \right] = 0$$

$$K_c = \frac{C_C^3}{C_A}$$

$$C_C = \frac{F_{A0}(3X)}{V_0(1+\epsilon X)}$$

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

$$\text{pure A} \rightarrow \theta_C = \frac{C_C}{C_A} = \frac{F_C}{F_A} = \frac{y_C}{y_A}$$

$$\Sigma = y_A \delta \quad 1 \times 2 = 2$$

$$C_C = \frac{C_{A0} 3X}{1+2X}$$

$$C_A = \frac{C_{A0}(1-X)}{(1+2X)}$$

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

0.25

$$C_{A0} = \frac{y_{A0} P_{A0}}{RT} = \frac{10 \times 1}{400 \times 0.082} = 0.3$$

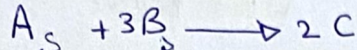
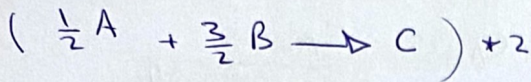
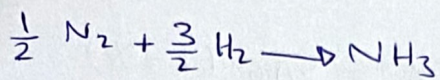
$$X = 0.25$$

$V = V_0$ constant

$$C_C = C_{A0} 3X$$

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

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



	inlet	change	
A	F_{A0}	$-F_{A0} X$	$F_A - F_{A0} X$
B	$F_{A0} \theta_B$	$-3X F_{A0}$	$F_{A0} (\theta_B - 3X)$
C	0	$+2X F_{A0}$	$F_{A0} (\theta_C + 2X)$

$$\theta_C = 0 \quad \text{if}$$

$$\theta_B = \frac{C_B}{C_A}$$

$$C_{A0} = \frac{P_0 y_A}{RT} = \frac{16.4 \times 0.15}{0.082 \times (227 + \frac{273}{T})}$$

$$\delta = 2 - 3 - 1 = -2$$

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

$$C_C = C_{A0} (\theta_C + X) \quad \nu = \nu_0$$

$$\frac{C_{A0} (\theta_C + X)}{1 + \varepsilon X}$$

ch4 1 design $\rightarrow$ ()

2 Rate law $\rightarrow -r_A = KC$

3 stoichiometry $\rightarrow C_A = \left(\frac{\quad}{\quad} \right)$

4 Combine.

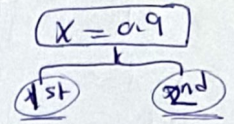
5 X, V, t, T

4.2 $\rightarrow$ 1 scal up
Batch R

$C_A \left\{ \begin{array}{l} t \end{array} \right.$

liquid or gas

example



$$1) N_{A0} \frac{dX}{dt} = -r_A$$

$$2) -r_A = KC_A$$

$$3) C_A = C_{A0} (1-X) \quad *$$

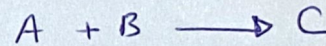
$$4) N_{A0} \frac{dX}{dt} = K C_{A0} (1-X)$$

$$\frac{dX}{dt} = \frac{K}{\nu_0} (1-X)$$

$$\int_0^X \frac{dX}{1-X} = \frac{K}{\nu_0} \int_0^t dt$$

$$-\ln(1-X) = \frac{K}{\nu_0} (t) \quad \text{L}$$

EX: - 4.1



$$C_{A0} = 2M$$

Batch

$$K = ?$$

time C_C

1 Batch

$$N_{A0} \frac{dX}{dt} = -r_A V$$

$$2) \text{rate} \Rightarrow -r_A = KC_A C_B$$

A	N_{A0}	$-N_{A0} X$	$N_{A0} (1-X)$
B	$N_{A0} \theta_B$	$-N_{A0} X$	$N_{A0} (\theta_B - X)$
C	0	$+N_{A0} X$	$N_{A0} X$

$$C_A = \frac{N}{V} = \frac{N_{A0} (1-X)}{\nu_0}$$

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

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

$$\frac{N_{A0}}{V} \frac{dX}{dt} = -r_A V$$

$$C_{A0} \frac{dX}{dt} = -r_A$$

$$\frac{dC_A}{dt} = -r_A$$

9

$$\frac{dCA}{dt} = r_A$$

$$\frac{dCA}{dt} = -KCA$$

$$\frac{dCA}{CA} = -K dt$$

$$\ln \frac{CA}{CA_0} = -Kt$$

$$C_c = \frac{CA_0}{\tau} X = CA_0 - CA$$

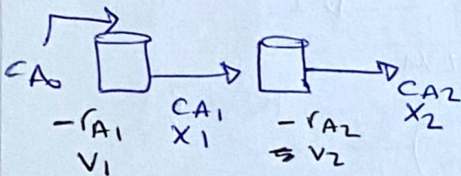
$$CA = CA_0 - C_c$$

$$\ln \frac{CA}{CA_0} = -Kt$$

• $\tau = \frac{V}{F_{A0}}$

4.22 Design CSTR

Series:-



$$CA_1 = ?$$

$$CA_1 = \frac{CA_0}{1 + \tau_1 K_1}$$

$$CA_2 = \frac{CA_1}{1 + \tau_2 K_2}$$

$$CA_n = \frac{CA_0}{(1 + \tau K)^n}$$

$n \rightarrow$ no. of reactor

$$V_1 = \frac{F_{A0} X}{-r_{A1}} = \frac{F_{A0} - F_{A1}}{K CA_1}$$

$$V_1 = \frac{V_0 (CA_0 - CA_1)}{K CA_1}$$

$$\tau K_1 CA_1 + CA_1 = CA_0$$

$$CA = CA_0 (1 - X)$$

$$CA_n = \frac{CA_0}{(1 + \tau K)^n}$$

$X \uparrow$

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

Series

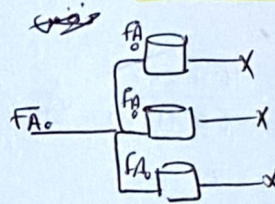
CSTR 1^{st} order - constant V

Parallel CSTR

$$V = V_1 + V_2 + V_3 + \dots$$

$$X_1 = X_2 = X_3$$

1^{st}



$$X = \frac{\tau K}{1 + \tau K}$$

$$V_i = F_{A0i} \cdot \left(\frac{X_i}{-r_{Ai}} \right)$$

$$V_i = \frac{V_T}{n} \rightarrow \text{no. reactor.}$$

$$F_{A0i} = \frac{F_{AT}}{n} \rightarrow \text{no. reactor.}$$

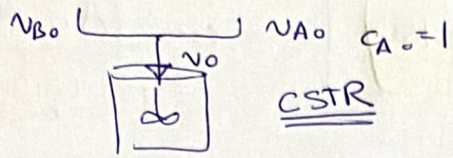
$$\frac{V}{n} = \frac{F_{A0}}{n} \left(\frac{X_i}{-r_{Ai}} \right)$$

2^{nd}

$$X = \frac{(1 + 2Da) - \sqrt{1 + 4Da}}{2Da}$$

$$Da = K CA_0 \tau$$

4.2



$$V_0 = V_{A0} + V_{B0}$$

(a) $V = ?$ $X = 0.8$
 $\dot{m} = 200 \times 10^6 \text{ (c)}$
 $K = 0.311 / \text{min}$

(1) Design $V = \frac{F_{A0} X}{-r_A}$

(2) $-r_A = K C_A$

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

(4) combine

$$V = \frac{F_{A0} X}{K C_{A0} (1 - X)}$$

$$V = \frac{V_0 X}{K (1 - X)}$$

$$V_0 = 2 V_{A0}$$

$$V_{A0} = \frac{F_{A0}}{C_{A0}}$$

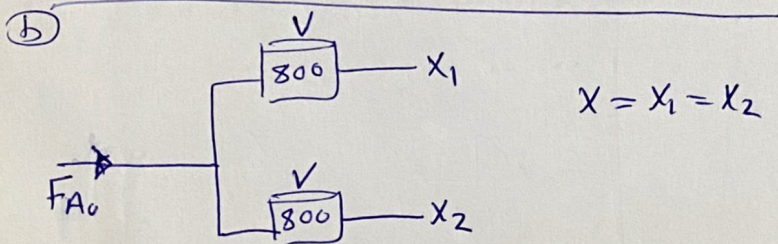
$C, A_{\text{con}} \rightarrow \text{concentration}$

$$F_C = F_{A0} X \rightarrow 0.8$$

$$F_C = 200 \times 10^6 \times \frac{1}{62}$$

$$F_C = 6.137$$

$$V = \frac{15.34 \times 0.8}{0.311 (1 - 0.8)} = 197.3$$



$X = ?$
 1st

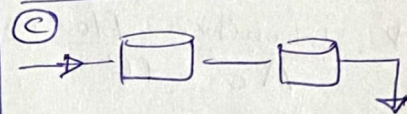
$$X = \frac{\tau K}{1 + \tau K}$$

$$\tau = \frac{V}{V_0} = \frac{800}{V_0}$$

$$V_0 = \frac{V_0 \tau}{\tau} = \frac{15.34}{2} = 7.67$$

$$\tau = 13.94 \text{ min}$$

$$X = \frac{\tau K}{1 + \tau K} = 0.81$$

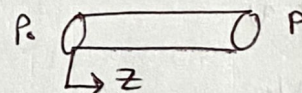


$$X = 1 - \frac{1}{(\tau K + 1)^n}$$

$$X = 1 - \frac{1}{(2.16 - 1)^2} = 0.9$$

$$\tau = \frac{V}{V_0} = \frac{800}{15.3 \times 7.68} = 6.97$$

Pressure drop in Reactors



gas phase $\rightarrow$ gas phase

$$C_i = \frac{F_i}{V_B} = \frac{C_A (\theta P + V_i X)}{(1 + \epsilon X) \left(\frac{P}{P_0} \right)^{\frac{1}{1 + \epsilon X}}}$$

PBR $A \rightarrow B + C$

(1) $F_{A0} = \frac{dX}{dW} = -r_A$

(2) $-r_A = K C_A^2$

(3) $C_A = \frac{C_{A0} (1 - X)}{(1 + \epsilon X) \left(\frac{P}{P_0} \right)^{\frac{1}{1 + \epsilon X}}}$

هذا هو

$$\frac{dX}{dW} = \frac{K C_{A0} \left(\frac{1 - X}{1 + \epsilon X} \right)^2 \left(\frac{P}{P_0} \right)^{\frac{2}{1 + \epsilon X}}}{1}$$

هذا هو

(10)

$$\frac{dP}{dz} = \frac{-G}{g_c f D_p} * \frac{(1-\phi)}{\phi^3} \left[\frac{150(1-\phi)\mu}{D_p} + 1.75G \right]$$

$$W = \underbrace{A_c * z}_{\text{volume bed}} * \underbrace{f}_{\text{volume solid}} \frac{V_{\text{solid}}}{V_{\text{bed}}}$$

$P \rightarrow$ Pressure

$\phi \rightarrow$ Porosity = $\frac{V_{\text{voids}}}{V_{\text{tot bed}}}$

$$(1-\phi) = \frac{V_{\text{solid}}}{V_{\text{tot bed}}}$$

$$g_c = 32.174 \text{ } \frac{\text{lbm}}{\text{ft} \cdot \text{s}^2}$$

$$D_p = \text{ft}$$

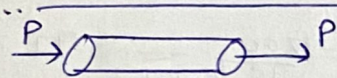
$\mu \rightarrow$ viscosity gas

$$u \rightarrow \frac{\text{Volumetric flow rate}}{A_c} \frac{\text{ft}^3/\text{h}}{\text{ft}^2}$$

$$\frac{\text{ft}}{\text{hr}}$$

$$G = \rho * u$$

$$\frac{\text{g}}{\text{cm}^3 \cdot \text{s}} \quad \frac{\text{lbm}}{\text{ft}^3 \cdot \text{h}}$$



In = out (mass)

$$\dot{m}_{\text{in}} = \dot{m}_{\text{out}}$$

$$\rho_0 V_0 = \rho V$$

$$\rho = \frac{\rho_0 V_0}{V} \rightarrow V_0 \frac{\rho_0}{\rho} \frac{T}{T_0} \frac{F_T}{F_T}$$

$$\rho = \rho_0 \frac{V_0}{V} * \frac{P}{P_0} * \frac{T}{T_0} * \frac{F_{T_0}}{F_T}$$

$$\left(\beta_0 = \frac{G(1-\phi)}{\rho_0 g_c} \right) \text{ } \frac{\text{lbm}}{\text{ft}^3 \cdot \text{s}^2}$$

$$\frac{dP}{dz} = \beta_0 \frac{\rho_0}{\rho} * \frac{T}{T_0} \frac{F_T}{F_{T_0}}$$

بسی ایئر کما

$$\rho_b = \frac{\text{Solid mass}}{V_{\text{reactor}}}$$

$$\rho_s = \frac{\text{solid mass}}{V_{\text{solid}}}$$

$$\rho_b = (1-\phi) \rho_s$$

$$dW = A_c * f * (1-\phi) * dz$$

$$dz = \frac{dW}{A_c f (1-\phi)}$$

$$\frac{dP}{dW} = \frac{-\beta_0}{A_c (1-\phi) f} \frac{P_0}{P} \frac{T}{T_0} \frac{F_T}{F_{T_0}}$$

$$\alpha = \frac{2\beta_0}{A_c f (1-\phi) P_0} = \frac{2\beta_0 z}{W}$$

$$\frac{dP}{dW} = -\frac{\alpha}{2} \frac{T}{T_0} \frac{P_0}{P/P_0} (1 + \epsilon x)$$

$$\frac{P}{P_0} = (1 - \alpha W)^{0.5}$$

$$\frac{P}{P_0} = \left(1 - \frac{2\beta_0 z}{P_0} \right)^{0.5}$$

Scanned with

(4.6 example)



$x = 0.6$, $w = ??$
weight

$K = 0.0141 \frac{\text{lbmol}}{\text{atm}^{1/3} \text{ h}}$

$$-r_A' = K (P_A^{1/3}) (P_B)^{2/3}$$

Solution

$C_A = \frac{P_A}{RT} \rightarrow P_A = C_A RT$
 $P_B = C_B RT$

عاري جوعه

① $F_{A0} \frac{dx}{dw} = -r_A'$

② $-r_A' = K (C_A RT)^{1/3} (C_B RT)^{2/3}$
 $-r_A' = K RT C_A^{1/3} C_B^{2/3}$

③ $C_A = \frac{C_{A0} (1-x)}{(1+\epsilon x)} \frac{P}{P_0}$

$C_B = \frac{C_{A0} (1 - \frac{1}{2}x)}{(1+\epsilon x)} \frac{P}{P_0}$

$\Theta_B = \frac{F_{B0}}{F_{A0}} = 1/2/1 = 1/2$

$C_B = \frac{C_{A0} (1 - \frac{1}{2}x)}{(1+\epsilon x)} \frac{P}{P_0}$

$-r_A' = K RT \left(\frac{C_{A0} (1-x)}{(1+\epsilon x)} \frac{P}{P_0} \right)^{1/3} \left(\frac{C_{A0} (1/2 - 1/2x)}{(1+\epsilon x)} \frac{P}{P_0} \right)^{2/3}$

هلا بي افتر و ادور على الحركه

$-r_A' = K RT C_{A0} \frac{(1-x)}{(1+\epsilon x)} \frac{P}{P_0} * (1/2)^{2/3}$
 $(K' = P_{A0}^{1/3} K)$

$-r_A' = K' \frac{(1-x)}{(1+\epsilon x)} \left(\frac{P}{P_0} \right)$

$-r_A' = \frac{K' (1-x)}{(1+\epsilon x)} (1-\alpha w)^{0.5}$

① هلا جوعه با

$F_{A0} \frac{dx}{dw} = \frac{K' (1-x)}{(1+\epsilon x)} (1-\alpha w)^{0.5}$

$\int_0^w (1-\alpha w)^{0.5} dw = \int_0^x \frac{F_{A0} (1+\epsilon x)}{K' (1-x)} dx$

$\Rightarrow w = 1 - \left[1 - \left(\frac{3\alpha F_{A0}}{2K'} (1+\epsilon x) \ln \left(\frac{1}{1-x} \right) \right)^{2/3} \right]$

! $\alpha = \epsilon, K', \epsilon$

④ $\epsilon = y_{A0} \delta = \frac{F_{A0}}{F_{T0}} \delta = \frac{0.3 * 10^{-3}}{1}$

$F_{A0} + F_{B0} + F_{T0}$

$\frac{0.79}{0.21} \frac{M_2}{M_1}$

$y = \frac{1.08}{3.65} = 0.3$

$\epsilon = 0.3 * (1 - \frac{1}{2} - 1) = -0.15$

$K' = K P_{A0} (1/2)^{2/3}$

$P_{A0} = y_{A0} P_0 = 0.3 * 10 = 3$

$K' = 0.0266$

$\alpha = \frac{2\beta_0}{A_c (1-\phi) \rho * P_0}$ given β_0

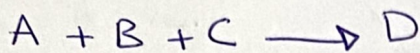
$\beta_0 = \frac{G(1-\phi)}{\rho_0 g_c D_p \phi^2} \left[\frac{150(1-\phi) \mu}{D_p} + 1.75 G \right]$

$G = \rho u = \frac{\dot{m}_T}{A_c} = \frac{\dot{m}_A + \dot{m}_B + \dot{m}_C}{A_c}$

Collection and analysis of Rate Data

Method of Excess

order of success



(Isolation method)

(reactant) - $\frac{1}{\alpha-1}$

[A] [B] [C]

Rate

$$\text{order} = \frac{\frac{\text{rate}^2}{\text{rate}^1}}{\frac{[A]^2}{[A]^1}}$$

Example $A + B + 2C \rightarrow D + 2E$

[A]	[B]	[C]	rate
0.1	0.5	0.25	0.1
0.2	0.5	0.25	0.2

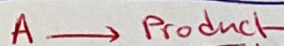
$$\text{order} = \frac{0.2}{0.1} = 1$$

$$\text{order} = \frac{0.8}{0.1} = 2$$

$$\text{order} = \frac{0.2}{0.1} = 2$$

$$-r = k C_A^1 C_B^2 C_C^2$$

Half-Life Method



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

$$-\frac{dC_A}{dt} = -r_A$$

$$-\frac{dC_A}{dt} = k C_A^\alpha$$

$$\int_{C_{A0}}^{C_A} \frac{-dC_A}{C_A^\alpha} = \int_0^t -k dt$$

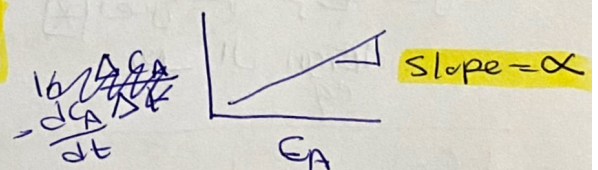
$$\frac{1}{\alpha-1} * \left(\frac{1}{C_A^{\alpha-1}} + \frac{1}{C_{A0}^{\alpha-1}} \right) = kt$$

$$t = \frac{1}{k C_{A0}^{\alpha-1} (\alpha-1)} \left[\left(\frac{C_{A0}}{C_A} \right)^{\alpha-1} - 1 \right]$$

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

$$-\frac{dC_A}{dt} = k C_A^\alpha$$

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

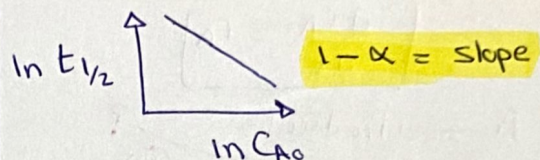


$$\frac{1}{3} \quad \frac{1}{8} \quad \frac{1}{2} \quad \text{اذابى انكر من}$$

$$t_{1/n} = \frac{n^{\alpha-1} - 1}{k(\alpha-1)} \left(\frac{1}{C_{A0}^{\alpha-1}} \right)$$

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

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



$$k = \frac{1}{[A] t_{1/2}}$$

Integral Method

Zero order	1st order	2nd order
rate = k	rate = k[A]	rate = k[A] ²
$[A]_t = [A]_0 - kt$	$\ln[A]_t = \ln[A]_0 - kt$	$\frac{1}{[A]_t} = \frac{1}{[A]_0} + kt$
$C_A = C_{A0} - kt$	$\ln C_A = \ln C_{A0} - kt$	$\frac{1}{C_A} = \frac{1}{C_{A0}} + kt$
slope = -k	slope = -k	slope = k

Differential Method

Ch5 :-

* Differential → order ١

* Integral → guess

* least square

Differential

$$N_A = C_A V$$

Batch $\Rightarrow \frac{dN_A}{dt} = A r_A V$

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

$$\boxed{\frac{dC_A}{dt} = r_A}$$

A — Product.

$$r_A = K C_A^\alpha$$

$$\frac{dC_A}{dt} = K C_A^\alpha$$

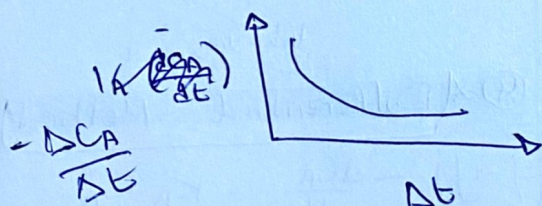
$$\ln\left(-\frac{dC_A}{dt}\right) = \ln K + \alpha \ln C_A$$

intercept slope

C_A	
Time	

(Data) في Δt

Diff — graph → Δt في t
 Num' → Δt في t



نقص الـ Δt بزيادة Δt
 sign الـ Δt

$$\int \frac{dC_A}{C_A^{\text{order}}} \Rightarrow \frac{1}{C_A^{\text{order}-1}} \star \frac{1}{(\text{order}-1)} \left(\frac{1}{C_A} \right) \Rightarrow \frac{1}{C_A^2}$$

* time — Integral — Δt

time			
C_A			
$\frac{dC_A}{dt}$	()	()	()

مقدار Δt

$$\frac{dC_A}{dt} = -3 C_{A0} +$$

Integral

A — Production

Batch Δt

(- $r_A = K$ Zero order)

$$\boxed{\frac{dC_A}{dt} = -K}$$

Zero Δt



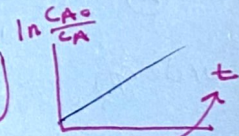
First order

$$-r_A = K C_A^1$$

$$\frac{dC_A}{dt} = -K C_A$$

$$\frac{dC_A}{C_A} = -K dt$$

$$\boxed{\ln \frac{C_{A0}}{C_A} = +Kt}$$



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

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

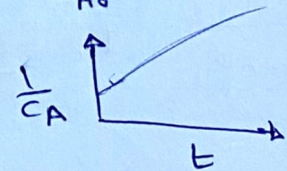
Second order

$$-r_A = K C_A^2$$

$$\frac{dC_A}{dt} = -K C_A^2$$

$$\frac{dC_A}{C_A^2} = -K dt$$

$$\frac{1}{C_A} - \frac{1}{C_{A0}} = Kt$$



* Applications of the Design Equations for continuous flow reactors

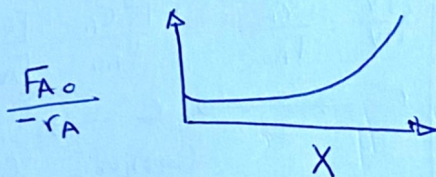
$$-r_A = f(X)$$

plot $\rightarrow \frac{F_{A0}}{-r_A}$ or $\frac{1}{-r_A}$ x axis $\rightarrow X$

of the plot $\Rightarrow$ $\frac{F_{A0}}{-r_A}$, $X \Rightarrow$ **Volume**
 PFR CSTR

irreversible reaction * * *
 order > 0
 * $X \uparrow$ $\rightarrow$ complete $x=1$

$X \rightarrow 1$ / $-r_A \rightarrow 0$
 Conversion $\downarrow$
 $V \rightarrow \infty$



reversible reaction * * *

max Conversion $\rightarrow$ equilibrium Conversion
 reaction rate $= 0$
 $-r_A = 0$

$X \rightarrow X_e$
 equilibrium

$-r_A \rightarrow 0$

$\frac{1}{-r_A} \rightarrow \infty$ $V \rightarrow \infty$

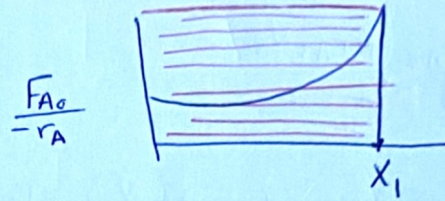
* $\frac{F_{A0}}{-r_A}$ $\rightarrow$ ∞ *
 * $\frac{1}{-r_A} \rightarrow \infty$ *
 * $V \rightarrow \infty$ *

CSTR

Volume ?

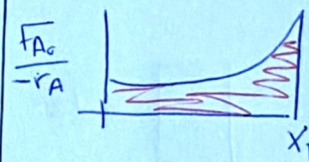
$$V = \frac{F_{A0} X}{-r_A}$$

$$V = \left(\frac{F_{A0}}{-r_A} \right)_{X_1} X_1$$



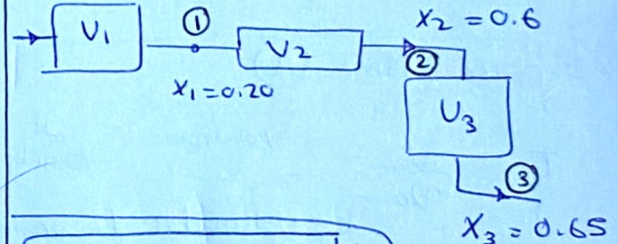
PFR

$$V = \int_0^{X_1} \frac{F_{A0}}{-r_A} dX$$



CSTR

PFR



* **Reactors in Series** *

(١) $X =$ total moles A reacted up to point i

$X =$ total moles A reacted up to point i
 moles A fed to first reactor.

(reactor 1)

* (NO side streams) *
 * (NO side streams) *

molar flow rate:-

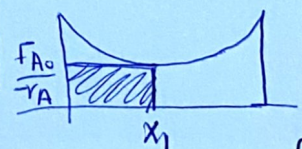
$$F_{Ai} = F_{A0} - F_{A0} X_i$$

Reactor 1 $\rightarrow$

$$F_{A1} = F_{A0} - F_{A0} X_1$$

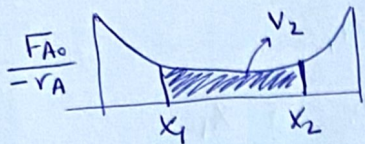
$$V_1 = \frac{F_{A0} - F_{A1}}{-r_{A1}} = \frac{F_{A0} - (F_{A0} - F_{A0} X_1)}{-r_{A1}}$$

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



Reactor ②

$$V_2 = \int_{x_1}^{x_2} \frac{F_{A0}}{-r_A}$$



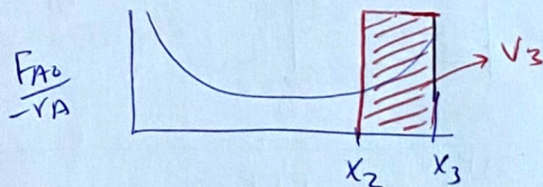
Reactor ③

$$F_{A2} - F_{A3} + r_{A3} V_3 = 0$$

(In - out) + gen = 0

$$(F_{A0} - F_{A0} x_2) - (F_{A0} - F_{A0} x_3) + r_{A3} V_3 = 0$$

$$V_3 = \frac{F_{A0} (x_3 - x_2)}{-r_{A3}}$$



Space Time (τ)

$$\tau = \frac{V}{V_0} \rightarrow \text{volume reactor} / \text{Volumetric flowrate}$$

avg. time $\frac{1}{\tau}$ reactor

Space Velocity

$$SV = \frac{V_0}{V} \quad SV = \frac{1}{\tau}$$

* Liquid hourly space velocity LHSV

$$LHSV = \frac{V_{0\text{liquid}}}{V}$$

* Gas - hourly space velocity GHSV

$$GHSV = \frac{V_0 \text{ at STP}}{V} \quad \text{Standard Temp. Pressure}$$

... 2 ...

* mde balance

PFR

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

CSTR

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

Batch

$$\frac{dx}{dt} = \frac{-r_A}{N_{A0}}$$

* rate laws

$$-r_A = K C_A$$

$$-r_A = \frac{K C_A}{1 + K_A C_A}$$

$$-r_A = K \left(C_A - \frac{C_R}{K} \right)$$

* Stoichiometry

(Flow)

$$C_A = \frac{F_A}{V}$$

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

liquid $V = V_0$

gas $V = V_0 (1 + \epsilon X) \frac{P_0 T}{P T_0}$

$$V = V_0$$

$$V = V_0 (1 + \epsilon X) \frac{P_0 T}{P T_0}$$

$$C_A = C_{A0}$$

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

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

(Batch)

$$C_A = \frac{N_A}{V}$$

$$N_A = N_{A0} (1 - X)$$

$$\text{gas } V = V_0 (1 + \epsilon X) \frac{P T}{P T_0}$$

$$\text{liquid } V = V_0$$

* Combine

$$\frac{dx}{dV} = \frac{-r_A}{F_{A0}} = \frac{K C_A}{F_{A0}} = \frac{K}{F_{A0}} \left(C_{A0} \frac{(1 - X)}{(1 + \epsilon X)} \right) \frac{P T_0}{P T}$$

$$r \rightarrow C \rightarrow X$$

Function Function

$$\frac{dx}{dV} = \frac{K}{V_0} \frac{(1 - X)}{(1 + \epsilon X)} y \frac{T_0}{T} \quad (y = \frac{P}{P_0})$$

$$V = \frac{V_0}{K} \left[(1 + \epsilon) \ln \left(\frac{1}{1 - X} \right) - \epsilon X \right]$$

Chs

example



Feed

Volumetric flowrate $v_0 = 0.0033 \frac{dm^3}{s}$

Acetic Anhydride 7.8% (1M)

Water 92.2% (51.2M)

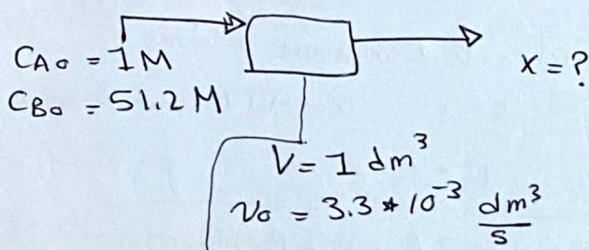
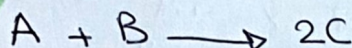
Elementary with $K = 1.95 \times 10^4 \frac{dm^3}{mol \cdot s}$

Case 1 $\rightarrow$ CSTR $\rightarrow V = 1 dm^3$

Case 2 $\rightarrow$ PFR $\rightarrow V = 0.311 dm^3$

(Conversion) x بدیے اعرف ادینی

CSTR



بدیے نصی باکی طوار

1 Mole Balance

CSTR

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

design equation

2 Rate Law

elementary

$$-r_A = K A C_A C_B$$

3 Stoichiometry

A	F_{A0}	$-F_{A0} X$	$F_A = F_{A0} (1-X)$
B	$F_{A0} \theta_B$	$-F_{A0} X$	$F_B = F_{A0} (\theta_B - X)$
C	0	$2 F_{A0} X$	$F_C = 2 F_{A0} X$

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

$$C_B = \frac{F_B}{v_0} = \frac{F_{A0} (\theta_B - X)}{v_0} = C_{A0} (\theta_B - X)$$

$$\theta_B = \frac{51.2}{1} = 51.2 \quad \frac{C_{B0}}{C_{A0}} = \theta_B$$

$$C_B = C_{A0} (51.2 - X) \approx C_{A0} (51.2) \approx C_{B0}$$

assumption

* invariable $\rightarrow (X \rightarrow 1)$

rate

r

هلا بجو صال (4)

$$-r_A = \underbrace{K' C_{B0}}_K C_{A0} (1-X)$$

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

هلا بجو صال (5)

$$V = \frac{F_{A0} X}{-r_A} \rightarrow v_0 C_{A0}$$

$$\rightarrow K C_{A0} (1-X)$$

$$V = \frac{v_0 C_{A0} X}{-K C_{A0} (1-X)}$$

$$\frac{V}{v_0} = \frac{X}{K (1-X)}$$

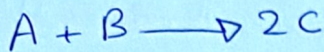
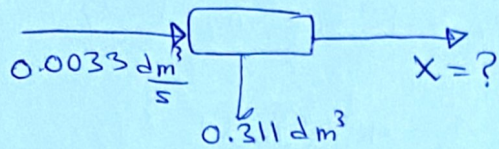
$$\tau = \frac{V}{v_0} = \frac{X}{K (1-X)}$$

$$X = \frac{\tau K}{1 + \tau K}$$

$$X = \frac{3.03}{4.03} = 0.75$$

مقابلة
Conversion
(1) τ

PFR ← example نفس



(Conversion) نسبة التحويل

1) Mole Balance

reactor ←

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

2) rate law

$$-r_A = K C_A C_B$$

3) Stoichiometry

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

$$C_B \approx C_{B0}$$

liquid phase

نفس قبل
بالمعدل

4) Combine

المجموع C بال T

$$-r_A = K' C_{B0} C_{A0} (1-X) = K C_{A0} (1-X)$$

$$\frac{dX}{dV} = \frac{K C_{A0} (1-X)}{C_{A0} V_0} \rightarrow \frac{dX}{dV} = \frac{K (1-X)}{V_0}$$

$$\int_0^X \frac{dX}{(1-X)} = \frac{K}{V_0} \int_0^V dV = K \tau$$

$$\ln \frac{1}{1-X} = K \tau$$

$$X = 1 - e^{-K\tau}$$

حاسبة بال T
و بال T

$$\tau = \frac{V}{V_0} = \frac{0.311 \text{ dm}^3}{0.0033 \text{ dm}^3/\text{sec}} = 94.2 \text{ sec}$$

$$X = 0.61$$

$$K = 0.015^{-1}$$

Zero ↑ order ← CSTR ×

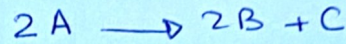
↑ Volume

$$3 V_{\text{CSTR}} = V_{\text{PFR}}$$

$$\text{CSTR} \Rightarrow V = \frac{F_{A0} (X_2 - X_1)}{-r_A}$$

$$\text{PFR} \Rightarrow V = \int_{X_1}^{X_2} \frac{F_{A0} dX}{-r_A}$$

example 2



$$C_A = 0.2 \text{ mol/dm}^3$$

$$K = 0.29 \text{ dm}^3/\text{mol.s}$$

$$\text{PFR} : \rightarrow V_0 = 10 \text{ dm}^3/\text{s}$$

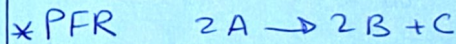
$$\tau = ? \quad X = 0.9$$

$$V = ? \quad X = 0.9$$

Batch → Constant Volume.

$$t = ? \quad X = 90\%$$

$$\tau = ?$$



$$V_0 = 10$$

$$K = 0.29$$

$$C_{A0} = 0.2$$

$$T = T_0 \quad P = P_0 \quad X = 0.90 \quad V = ?$$

نفس الخطوات :-

1) Mole Balance :-

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

2) rate law → $-r_A = K C_A^2$

3) Stoichiometry

$$V = V_0 (1 + \epsilon X) \quad (\text{gas flow})$$

$$C_A = \frac{C_{A0} (1-X)}{1 + \epsilon X} \rightarrow A \rightarrow B + \frac{1}{2} C$$

$$\frac{P}{P_0} = 1 \quad \frac{T}{T_0} = 1$$

4) Combine

$$-r_A = \frac{K C_{A0}^2 (1-X)^2}{(1 + \epsilon X)^2}$$

* rate
* mole
Balance

$$\frac{dX}{dV} = \frac{K C_{A0}^2 (1-X)^2}{C_{A0} V_0 (1 + \epsilon X)^2}$$

* مقارنة
X و T

$$\int_0^X \frac{(1 + \epsilon X)^2}{(1-X)^2} dX = \int_0^V \frac{K C_{A0}}{V_0} dV$$

$$\frac{K C_{A0} V}{V_0} = K C_{A0} \tau = Da$$

Chs $K C_{A0} \tau = 2(1+\varepsilon) \ln(1-X) + \sum^2 X + \frac{(1+\varepsilon)^2 X}{1-X}$

mole fraction initial pure = 1

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

$K C_{A0} \tau = 17.02$

$\tau = \frac{17.02}{K C_{A0}} = 294 \text{ sec.}$

$V = v_0 \tau = 2940 \text{ L}$

$\sum \nu_i = \nu$
 $\left(\frac{1}{2} + 1\right) - 1 = \frac{1}{2}$

Batch:

① mole Balance:-

$\frac{dX}{dt} = \frac{-r_A V_0}{N_{A0}} = \frac{-r_A}{N_{A0}/V_0} = \frac{-r_A}{C_{A0}}$

② Rate Law:-

$-r_A = K C_A^2$

③ Stoichiometry (gas flow)

$V = V_0$

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

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

④ Combine

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

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

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

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

$t = 155 \text{ s}$

نفسه
 mole Balance
 same
 X, t

* Pressure Drop in (PBRs)

gas $\rightarrow$ يكون في تيار الغاز

وكانت عند constant

* Concentration Flow System:-

$C_A = \frac{F_A}{v}$

* gas Phase Flow System:-

$v = v_0 (1 + \varepsilon X) \frac{T}{T_0} \frac{P_0}{P}$

$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X) \frac{T}{T_0} \frac{P_0}{P}}$

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

$C_B = \frac{F_B}{v} = \frac{F_{A0}(\theta_B - \frac{b}{a} X)}{v_0(1+\varepsilon X) \frac{T}{T_0} \frac{P_0}{P}}$

$C_B = \frac{C_{A0}(\theta_B - \frac{b}{a} X) \frac{T_0 P}{T P_0}}{(1+\varepsilon X)}$

P drop $\xrightarrow{\text{gas phase}} \text{liquid phase}$

* example

Second order gas phase reaction isothermally PBR



① Mole Balances (PBR)

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

② Rate Laws

$-r_A = K C_A^2 \rightarrow \text{second order}$

③ Stoichiometry

$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X) \frac{P}{P_0} \frac{T_0}{T}}{(1+\varepsilon X)}$

isothermal $T = T_0$

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

Ch 5

isothermal system

isothermal system

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

isothermal system example

$$\frac{dX}{dw} = \frac{K C_A^2 (1-X)^2}{F_{A0} (1 + \epsilon X)^2} y^2$$

$$\frac{dX}{dw} = f(X, P)$$

$$\frac{dP}{dw} = f(X, P) \quad \text{or} \quad \frac{dy}{dw} = f(y, X)$$

⊗

* Packed Bed Reactors

$$\epsilon = 0$$

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

$$W = 0 \rightarrow y = 1$$

$$dy^2 = -\alpha dw$$

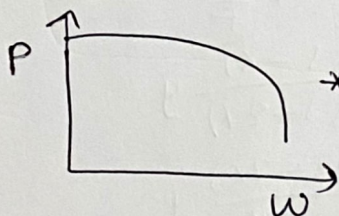
$$y^2 = (1 - \alpha w)$$

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

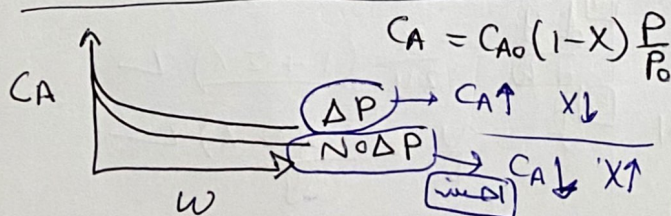
بداية
Catalyst
 $y = 1 = \frac{P}{P_0}$

Space
Space
Case

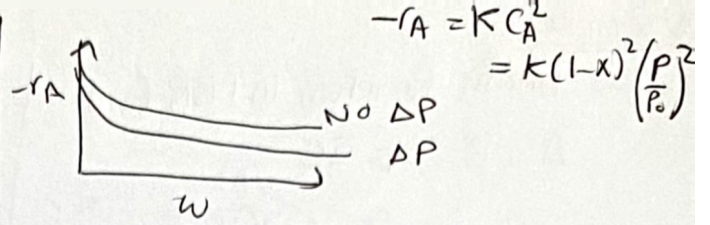
isothermal + $\epsilon = 0$



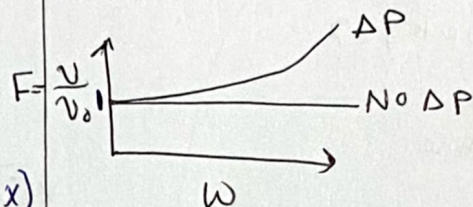
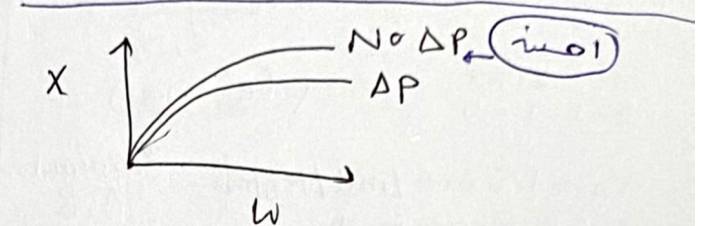
* Pressure Drop PBR



$$C_A = C_{A0} (1-X) \frac{P}{P_0}$$



$$-r_A = K C_A^2 = K (1-X)^2 \left(\frac{P}{P_0}\right)^2$$



Flow rate in PBR

$$\epsilon = 0 \quad v = v_0 \left(\frac{P_0}{P}\right)$$

$F \uparrow \leftarrow \downarrow \Delta P$
 $\epsilon \rightarrow \text{flow}$
 $\downarrow \text{Time}$

$$v = v_0 (1 + \epsilon X) \frac{P_0}{P} \frac{T}{T_0}$$

$$T = T_0$$

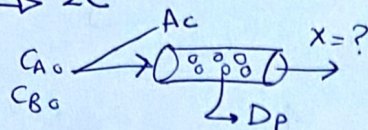
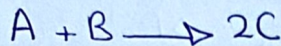
$$y = \frac{P_0}{P}$$

$$f = \frac{v_0}{v} = \frac{1}{(1 + \epsilon X) y}$$

isothermal

*Example

Gas Phase Reaction in PBR for $\delta=0$



$$\Delta S = 0$$

$$2 - 1 - 1 = 0$$

$$K_A = 1.5 \text{ dm}^3 / \text{mol} / \text{kg} / \text{min}$$

$$\alpha = 0.0099 \text{ kg}^{-1}$$

Find X at 100 kg ?

1 Mole Balance.

$$\frac{dX}{dW} = \frac{-r'_A}{F_{A0}}$$

2 Rate Law

$$-r'_A = K C_A C_B$$

3 Stoichiometry

$$C_A = C_{A0} (1-X) y \rightarrow \frac{P}{P_0}$$

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

$$\left[\begin{aligned} \frac{dy}{dW} &= -\frac{\alpha}{2y}, \quad 2y dy = -\alpha dW \\ W=0 \quad y=1 \quad y^2 &= 1-\alpha W \\ y &= (1-\alpha W)^{1/2} \end{aligned} \right]$$

4 Combine

$$\begin{aligned} -r_A &= K C_{A0}^2 (1-X)^2 y^2 \\ &= K C_{A0}^2 (1-X)^2 (1-\alpha W) \end{aligned}$$

$$\frac{dX}{dW} = \frac{K C_{A0}^2 (1-X)^2 (1-\alpha W)}{F_{A0}}$$

W, X, L

integration

$$\frac{dX}{(1-X)^2} = \frac{K C_{A0}^2}{F_{A0}} (1-\alpha W) dW$$

$$\frac{X}{1-X} = \frac{K C_{A0}^2}{F_{A0}} \left(W - \frac{\alpha W^2}{2} \right)$$

$$W=0$$

$$X=0$$

$$W=W$$

$$X=X$$

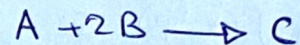
$$X = 0.6 \text{ with } P \text{ drop}$$

$$X = 0.75 \text{ without } P \text{ drop}$$

$$\alpha=0$$

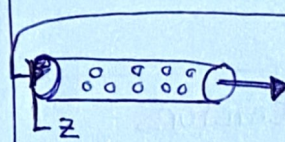
$\downarrow X$ $\leftarrow$ $P \text{ drop}$
 $F \uparrow$

*Example



$$\delta \neq 0$$

$$\begin{aligned} P_0 &= 10 \text{ atm} \\ F_{A0} &= 2 \text{ mol/min} \\ C_{A0} &= 0.2 \text{ mol/dm}^3 \end{aligned}$$



$$y = \frac{P}{P_0}$$

Stoichiometric

$$\frac{F_{A0}}{C_{B0}} = \frac{1}{2} \rightarrow \text{Plot } X + P \text{ ratio } y = \frac{P}{P_0}$$

$$K_A = 6$$

$$\alpha = 0.02$$

Weight Catalyst
100 kg

1 Mole Balance

$$\frac{dX}{dW} = \frac{-r'_A}{F_{A0}}$$

2 rate law

$$-r'_A = K C_A C_B^2$$

3 Stoichiometry (gas - isothermal)

$$V = V_0 (1 + \epsilon X) \frac{P_0}{P}$$

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

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

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

$$f = \frac{V}{V_0} = \frac{(1+\epsilon X)}{y}$$

$$\Sigma = y_{A_0} (1 - 1 - 2) = \frac{1}{2} - 2 = -\frac{2}{3}$$

$$C_{A_0} = 2, F_{A_0} = 2, K = 6, \alpha = 0.02$$

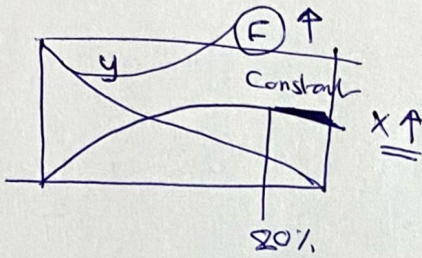
$$W = 0, X = 0, y = 1 \quad \underline{\text{initial}}$$

$$W = 100 \quad \underline{\text{final}}$$

$$\frac{1}{2+1}$$

$$\Sigma \neq 0$$

→ Polymath



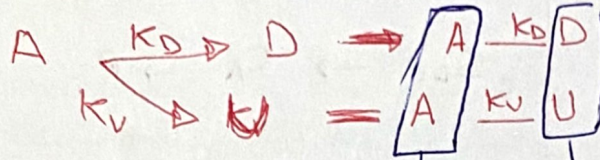
! Pressure Drop

Multiple Reaction

maximizes
الشيء الذي يري بيا

minimizes
الشيء الذي لا يري بيا

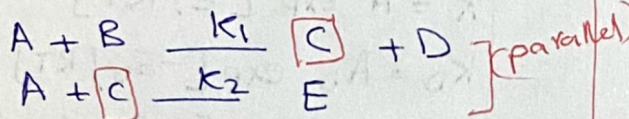
1) Parallel reaction



reactant استرکوا بال
product الناتج بال

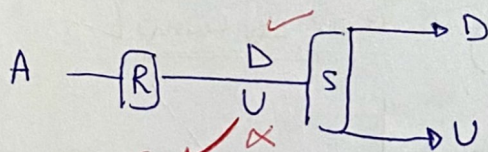
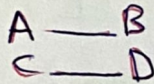
2) Series $H \xrightarrow{K_1} B \xrightarrow{K_2} C$

3) تفاعلين متتاليين (series + parallel)



intermediate component (series)

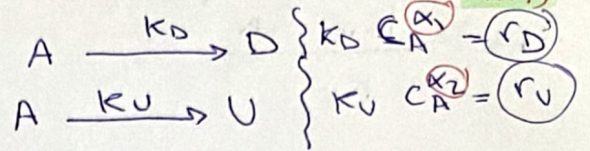
4) independent reaction



بدي اقل عدها
من مخرج مصدري
كي بالفضل
ويكون ال reaction
منبع اقتصادي

overall $\rightarrow F$
overall $\rightarrow r$

S.1 Maximization of D (parallel rxn)



$$\begin{aligned} -r_A &= r_D + r_U \\ &= K_D C_A^{\alpha_1} + K_U C_A^{\alpha_2} \end{aligned}$$

* Instantaneous selectivity

$$S_{DU} = \frac{\text{rate of formation D}}{\text{rate of formation U}}$$

$$S_{DU} = \frac{r_D}{r_U} = \frac{K_D C_A^{\alpha_1}}{K_U C_A^{\alpha_2}}$$

$$\left[\frac{S_{DU}}{S_{DU}} = \frac{K_D}{K_U} C_A^{\alpha_1 - \alpha_2} \right] \quad \#$$

* overall selectivity

$$\bar{S}_{DU} = \frac{\text{molar flowrate exit D}}{\text{molar flowrate exit U}}$$

$$\bar{S}_{DU} = \frac{F_D}{F_U} = \frac{N_D}{N_U} \quad (\text{batch})$$

* Instantaneous yield

$$y_D = \frac{\text{reaction Rate D}}{\text{reaction Rate A}}$$

$$y_D = \frac{r_D}{-r_A} = \frac{r_D}{r_D + r_U}$$

* overall yield

$$\bar{y}_D = \frac{F_D}{F_{A_0} - F_{A_1}}$$

$$= \frac{F_D}{F_{A_0} \cdot X}$$

(CSTR)

mol. formation
mol. of
limiting
reaching
consumed.

$$(\text{Batch}) \Rightarrow \bar{y}_D = \frac{N_D}{N_{A_0} - N_A}$$

Ch6
①

* 6.1.1

$$S_{DU} = \frac{K_D C_A^{\alpha_1 - \alpha_2}}{K_U}$$

کیفیت
بسیار زیاد

Case 1) $\alpha_1 > \alpha_2$

$$a = \alpha_1 - \alpha_2 = a \text{ (+ve)}$$

$$S_{DU} = \frac{K_D}{K_U} C_A^a$$

Concentration C_A

* کیفیت بزرگ، زیاد

* gas system rxn

$$C_A = \frac{P_{tot} y_A}{RT}$$

$S_{DU} \rightarrow C_A \rightarrow P$ ریاستی
تغییر

1) high P (gas system)

* liquid system rxn

2) (no dilution)

حاجت به اقل C_A
لایه بزرگ ازید

3) CSTR, batch, PFR

خارج انتقال

exit آلودگی

high concentration
بزرگ بقیه

(C_A بزرگ بقیه)

نقطه و اقل

Case 2) $\alpha_1 < \alpha_2 \Rightarrow a$

$$S_{DU} = \frac{K_D}{K_U} C_A^{-a}$$

$$S_{DU} = \frac{K_D}{K_U} C_A^a$$

$S_{DU} \rightarrow C_A \rightarrow P$

در یک گونه الک

کیفیت بزرگ

1) low P (gas)

2) liquid (use dilution)

3) CSTR ✓

$$K = A \exp[-E/RT]$$

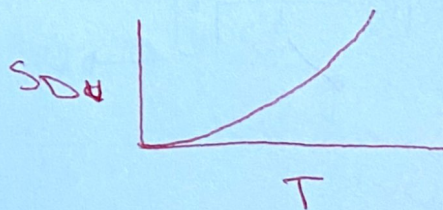
$$K_D = A_D \exp[-E_D/RT]$$

$$K_U = A_U \exp[-E_U/RT]$$

$$\Rightarrow \frac{K_D}{K_U} = \frac{A_D}{A_U} \exp\left[-\frac{E_D - E_U}{RT}\right]$$

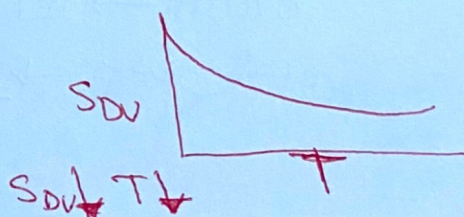
Case 3) $E_D > E_U$

max temp

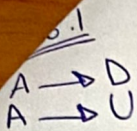


$S_{DU} \uparrow T \uparrow$

Case 4) $E_U > E_D$



$S_{DU} \downarrow T \downarrow$



gas phase.

$$r_D = 0.0012 \exp\left[\frac{K_D}{26000}\left(\frac{1}{300} - \frac{1}{T}\right)\right] C_A$$

$$r_U = 0.0018 \exp\left[\frac{K_U}{25000}\left(\frac{1}{300} - \frac{1}{T}\right)\right] C_A^{1.5}$$

Condition , reactor $\rightarrow$ maximum selectivity
 بحيث يكون عندك

$$S_{D/U} = \frac{r_D}{r_U} = 0.66 \exp\left[\frac{1000}{E_D - E_U}\left(\frac{1}{300} - \frac{1}{T}\right)\right] C_A^{-0.5}$$

$$S_{D/U} = 0.66 e^{1000\left(\frac{1}{300} - \frac{1}{T}\right)} \rightarrow \frac{1}{C_A^{0.5}}$$

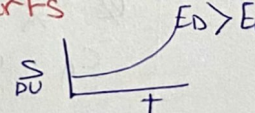
Case 2 $\rightarrow C_A^{0.5} \rightarrow$ بلعاق

Case 3 $\rightarrow E_D > E_U \rightarrow 1000$

1 $\downarrow$ low p $\rightarrow \downarrow C_A \rightarrow \downarrow P/U \uparrow$

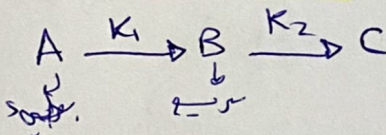
2 CSTR

3 dilute $\Rightarrow$ inerts

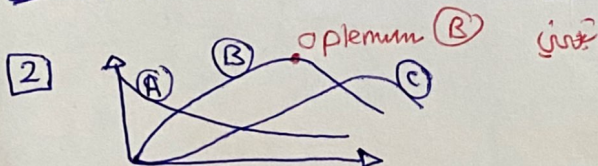
4 $\uparrow$ high Temp $\rightarrow$ 

$C_A \downarrow \rightarrow \uparrow S_{D/U}$

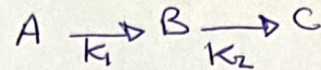
6.2 Series rxn



1 1st rxn slow
 2 2nd rxn fast $\rightarrow$ B يكون



6.3, 6.4



$$y_A = 0.1$$

$$\dot{V} = \dot{V}_0$$

concentration B = ? optimum.
 $C_{B \text{ opt}}?$

$$C_{B \text{ (opt)}} = C_{A0} (1 - X_{\text{opt}})$$

* العلاقة بين A و B و C

* mole balance.

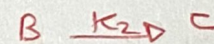
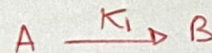
1

2

3

4

نقطة
 حرجية



PBR

$$\textcircled{1} \textcircled{A} \quad v_0 \frac{dC_A}{dW} = -r_A'$$

$$-r_A' = K_1 C_A$$

$$v_0 \frac{dC_A}{dW} = -K_1 C_A$$

$$v_0 \int_{C_{A0}}^{C_A} dC_A = -K_1 \int_0^W dW$$

تكامل

$$v_0 \ln \frac{C_A}{C_{A0}} = -K_1 W$$

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

$$PBR = \tau' = \frac{W}{v_0}$$

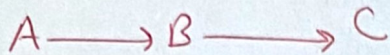
$$v_0 \ln \frac{C_A}{C_{A0}} = -K_1 \frac{W}{v_0} \rightarrow \tau'$$

$$C_A = C_{A0} e^{-K_1 \tau'}$$

τ' $\rightarrow$ C_A $\rightarrow$ τ'

$$\textcircled{B} \quad v_0 \frac{dC_B}{dW} = -r_B'$$

حرف ب انه $\frac{B}{C}$ عنده $\frac{B}{C}$



حرة كوست و حرة اسهل

$$(-r_B' = K_1 C_A - K_2 C_B)$$

$$v_0 \frac{dC_B}{dW} = K_1 C_A - K_2 C_B$$

عوضنا

$$v_0 \frac{dC_B}{dW} + K_2 C_B = K_1 C_{A_0} e^{-K_1 T}$$

$$T' = \frac{W}{v_0} \Rightarrow W = T' v_0$$

$$dW = dT' v_0$$

عوضنا

$$\frac{dC_B}{dT'} + K_2 C_B = K_1 C_{A_0} e^{-K_1 T'}$$

حلنا على طريقة integration method factor.



$$\frac{dy}{dx} + P(x)y = Q(x)$$

$$\textcircled{1} r(x) = \exp \int P(x) dx$$

$$\textcircled{2} y(x) = \left(\frac{1}{r(x)} \int r(x) Q(x) dx \right) + \frac{C}{r(x)}$$

$$\frac{dy}{dx} = \frac{-2}{x} y = x$$

$$\textcircled{1} r(x) = \exp \int \frac{-2}{x} dx = x^{-2}$$

$$\textcircled{2} y(x) = \left(\frac{1}{x^{-2}} \int x^2 x dx \right) + \frac{C}{x^{-2}}$$

$$y(x) = x^2 \ln x + x^2 C$$

بالاعادة عندي نبواستفاد

$$W=0 \quad T'=0$$

$$C_B=0$$

$$C_B = K_1 C_{A_0} \left[\frac{\exp^{-K_1 T'} - \exp^{-K_2 T'}}{K_2 - K_1} \right]$$

$$\frac{dC_B}{dT'} = 0$$

في استقر
اعماله في حرة

$$0 = \frac{K_1 C_{A_0}}{K_2 - K_1} \left(-K_1 e^{-K_1 T'} + K_2 e^{-K_2 T'} \right)$$

$$K_2 e^{-K_1 T_{opt}} = K_1 e^{-K_2 T_{opt}}$$

$$T_{opt} = \frac{1}{K_1 - K_2} \ln \frac{K_1}{K_2}$$

≠ *

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

$$X = \frac{C_{A_0} - C_A}{C_{A_0}}$$

$$= 1 - \frac{C_A}{C_{A_0}}$$

$$X_{opt} = 1 - e^{-K_1 T_{opt}}$$

طوبى
من
بعضها

بعضها

CSTR design

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

$$-r_A = K C_A$$

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

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

* كنا عوصنا ويطالع معنا وكتب V
Volume. ((const) ← T متغير)

هنا هو (T متغير)

RA و R(T) متغير

علاقة بين T و Conversion

$$K(T) = K(T_1) * \exp \left[\frac{E}{R} \left[\frac{1}{T_1} - \frac{1}{T} \right] \right]$$

initial دوبي ادبها

← K(T) بطوع

← RA بطوع

$$V = \frac{F_{A0} X}{K(T)}$$

$$K(T) = e \left(\frac{E}{R} * \left(\frac{1}{T_f} - \frac{1}{T} \right) \right) * C_{A0} (1-X)$$

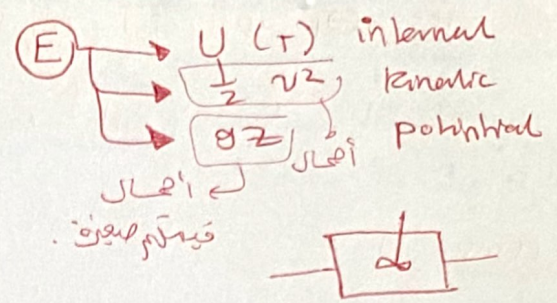
(liquid) ←

بجولين

بدي معادلة تانية فوق
اصولي

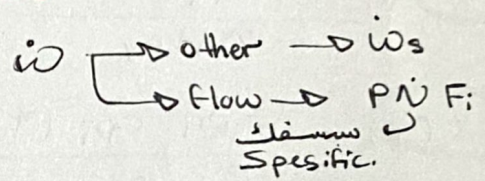
$$\frac{dE_{syst}}{dT} = E_{in} - E_{out}$$

Ch8
(1)



$$\frac{\partial E}{\partial t} = \dot{Q} - \dot{W} + \sum F_i E_i|_{in} - \sum F_i E_i|_{out}$$

Steady State. = 0



Flow work WF =

$$\dot{W}_F = \sum F_i P_i V_i|_{out} - \sum F_i P_i V_i|_{in}$$

$$\dot{W} = \dot{W}_s + \sum F_i P_i V_i|_{out} - \sum F_i P_i V_i|_{in}$$

$$\dot{Q} - \dot{W}_s + \sum F_i P_i V_i|_{in} + \sum F_i U_i|_{in} - \sum F_i P_i V_i|_{out} + \sum F_i U_i|_{out} = 0$$

$$\dot{Q} - \dot{W}_s + \sum F_i H_i|_{in} - \sum F_i H_i|_{out} = 0$$

$$\dot{Q} - \dot{W}_s + F_{A0} \sum Q_i (H_{i0} - H_i) - \Delta H_{Rxn} F_{A0} X = 0$$

$$\Delta H_{Rxn} = \Delta H_{Rxn}^0 + \Delta C_p (T - T_R)$$

reference.

$$\Delta H = c_{pi} (T - T_{i0})$$

$$\dot{Q} - \dot{W}_s - F_{A0} \left[\sum c_{pi} (T - T_{i0}) \right] - [\Delta H_{Rxn}^0 + \Delta C_p (T - T_R) F_{A0} X] = 0$$

$$Q - W_s - F_{A0} \sum \Theta_i C_{Pi} (T - T_s) - \Delta H_{Rx} F_{A0} X = 0$$

زنگنه اول سنی
بزدین بنشینو عن القند

$\Delta H_f + \Delta C_p \Delta T$

* temp + conversion *

$$\Delta C_p = 2 C_{p_{NH_3}} + 3 C_{p_{H_2}} -$$

$$= \text{يعطى لكن وحدة} \\ = -10.13 \text{ cal/mol}$$

$$\Delta H_{Rx} = -92.22 + (-10.12) (423 - 298)$$

$$* (3 \text{ كحول}) *$$

$$\dot{Q} = 0, \dot{W} = 0$$

$$\rightarrow \text{adiabatic} \text{ ①}$$

$$X = F(T)$$

$$X = \frac{\sum \Theta_i C_{Pi} (T - T_i)}{-\Delta H_{Rx}}$$

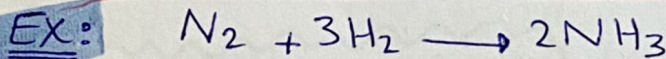
$$X(T) = \frac{\sum \Theta_i C_{Pi} (T - T_{i0})}{-\left[\Delta H_{Rx}^\circ + \Delta C_p (T - T_{ref})\right]}$$

$$T(X) = ?$$

$$Q = 0, W = 0$$

$$-F_{A0} \sum \Theta_i C_{Pi} T - F_{A0} \sum \Theta_i C_{Pi} T_{i0} \\ = -\Delta H_{Rx} * F_{A0} X - \Delta C_p F_{A0} X T \\ + \Delta C_p F_{A0} X T_{ref}$$

$$T = \frac{\Delta H_{Rx}^\circ X + \sum \Theta_i C_{Pi} T_{i0}}{\Delta C_p X - \sum \Theta_i C_{Pi}}$$



$$\Delta H_{Rx} = ?$$

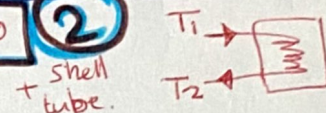
$$\Delta H_{Rx} = \Delta H_{Rx}^\circ + \Delta C_p (T - T_{ref})$$

$$\Delta H_{Rx}^\circ = 2 H_f(NH_3) - 0 - 0$$

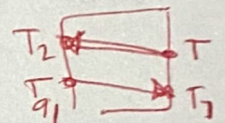
$$\dots O_2, N_2, H_2 \quad 0 = \text{العنصر في حالة مقاييسه} *$$

$$\Delta H_{Rx}^\circ = 2 * (-11020) \frac{\text{cal}}{\text{mol}} \\ = -92.22 \text{ kJ/mol}$$

$$* Q \neq 0 \text{ ②}$$



$$Q = U A \Delta T_{LM}$$



$$\Delta T_{LM} = \frac{T_{a1} - T_{a2}}{\ln \left(\frac{T - T_{a1}}{T - T_{a2}} \right)}$$

? out

$$T = T_{a1} = T_{a2}$$

$$\dot{m} C_p \Delta T_1 - \dot{m} C_p \Delta T_2 + \\ U A \frac{T_{a1} - T_{a2}}{\ln \left(\frac{T - T_{a1}}{T - T_{a2}} \right)} = 0$$

$$* \text{CSTR} \quad * \text{PFR}$$

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

$$-r_A = k C_A$$

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

فازي
first
order
+
liquid
phase

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

$$X = 0.5 \quad (V, T = ?) \text{ ممكن يعطى} *$$

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

Volume. وطلع

$$\Rightarrow V = 1000 \text{ gal.}$$

$$(X, T) = ?$$

$$\left. \begin{array}{l} \text{MB} \\ \text{EB} \end{array} \right\} \rightarrow X = f(T)$$

$$X_{MB} = f(T)$$

$$X_{EB} = f(T)$$

$$X_{EB} = \frac{\sum \Theta_i C_{pi} (T - T_{i0})}{\Delta H_{RX}} \quad \text{--- (1)}$$

$$V = \frac{F_{A0} X}{K(T) C_{A0} (1-X)}$$

معوضنا قيمتها

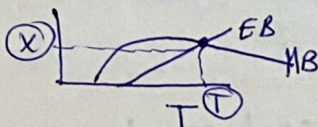
$$V = \frac{F_{A0} X}{K_{T1} \exp \left[\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \right] C_{A0} (1-X)} \quad \text{--- (2)}$$

CSTR
(Well mixed)

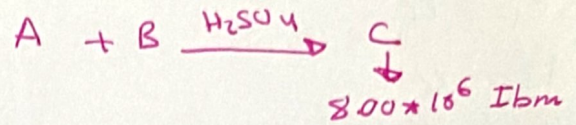
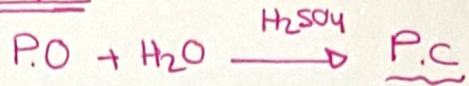


T	X _{EB}	X _{MB}
□	-	-
□	-	-
□	-	-

(برسم رسمة)



Example



$$F_{A0} = 43.04 \text{ lbmol/h}$$

$$V = 300 \text{ gal}$$

$$F_{A0} = 43.04 \text{ lbmol/h}$$

$$F_{M0} = 71.87 \text{ lbmol/h}$$

$$T = 58^\circ\text{F}$$

$$T = 56^\circ\text{F}$$

$$F_{B0} = 802.8 \text{ lbmol/h}$$

$$X = ?$$

$$T = ?$$

$$v_A = v_M = 46.62 \text{ ft}^3/\text{h}$$

$$v_B = 233.1 \text{ ft}^3/\text{h}$$

$$V = \frac{F_{A0} X}{-r_A} = \frac{F_{A0} X}{K(T) * C_{A0} (1-X)}$$

Liquid phase
mol Blank

$$V = \frac{v_0 X}{K(T) (1-X)}$$

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

$$\tau = \frac{X}{K(T) (1-X)}$$

$$\Rightarrow \left[X_{MB} = \frac{K(T) \tau}{1 + \tau K(T)} \right] \rightarrow \text{--- (1)}$$

معادلتين مع بعض بعض

او بكونه Graphical

$$\frac{X_{EB}}{1-X} = \frac{F_{A0} \sum \Theta_i C_{pi} (T - T_{i0}) - [\Delta H^0 + \Delta C_p (T - T_R)]}{-[\Delta H_{RXn} + \Delta C_p (T - T_R)]}$$

addabhtic

$F_{A0} X = 0$

$$X_{EB} = \frac{\sum \Theta_i C_{pi} (T - T_{i0})}{-[\Delta H_{RXn} + \Delta C_p (T - T_R)]} \rightarrow \text{--- (2)}$$

$$\sum \Theta_i c_{pi} = ??$$

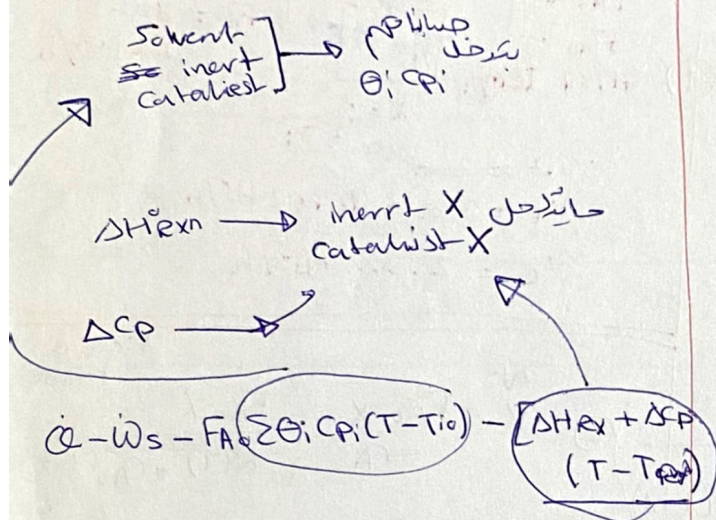
$$\Delta H_{rx} = ??$$

$$\Delta c_p = ??$$

$$T_{io} = ??$$

$$T_{ref} = ??$$

$$\tau = ?? \frac{V}{v_o}$$



$$\sum \Theta_i c_{pi} = \text{كل شيء داخل على (reactor)}$$

$$(c_{pA} \Theta_A + c_{pB} \Theta_B + c_{pM} \Theta_M)$$

$$\Theta_A = 1$$

$$\Theta_B = \frac{F_{Bo}}{F_{Ao}} = \frac{8022}{42} = ??$$

$$\Theta_M = \frac{F_{Mo}}{F_{Ao}} = \frac{72}{42} = ??$$

①

$$\sum \Theta_i c_{pi} = 403.3 \text{ Btu/lbmol F}$$

$$\Delta H_{rx} = H_{cp,c} (1) - H_{cp,c} (H_2O) - H_{cp,c} (H_2O)$$

داخل Inert لا يدخل بال rxn

$$(68 F) = (T_{ref})$$

$$\Delta H_{rx} = -364 \text{ Btu/lbmol F}$$

$$\Delta c_p = c_p (C) - c_p (B) - c_p (A)$$

$$= -7 \text{ Btu/lbmol F}$$

$$X_{EB} = 403.3 (T - 535)$$

$$R = \text{constant}$$

$$36400 + 7(T - (68 F + 460))$$

EB معادلة

$$\tau = \frac{V}{v_o} = \frac{300}{(46 + 23.1)} = 0.127 \text{ h}$$

$$X_{MB} = 0.123 * K(T) = ?$$

$$K(T) \exp \left(\frac{E}{R} * \left(\frac{1}{T} - \frac{1}{T_0} \right) \right)$$

$$1.987$$

$$K(T) = 16.96 * 10^{12} \exp \left(\frac{34400}{12T} \right)$$

في درجة حرارة

في درجة حرارة

في درجة حرارة

$$X_{MB} = 0.123 * 10^{12} * 16.96 \exp \left(\frac{-32400}{1.987 T} \right)$$

$$1 + 0.123 * 10^{12} * 16.96 \exp \left(\frac{-32400}{1.987 T} \right)$$

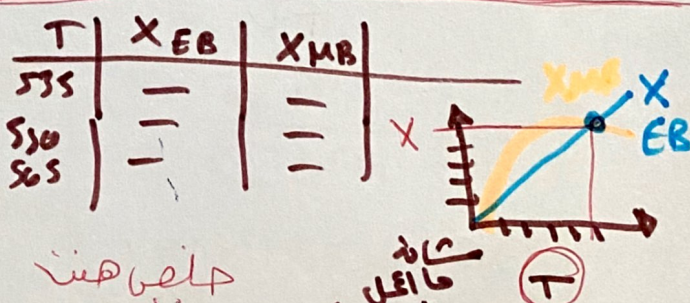
MB

* مع X EB

مع X EB

مع X EB

مع X EB



حاصل من

نظري

بالإضافة إلى

بالإضافة إلى

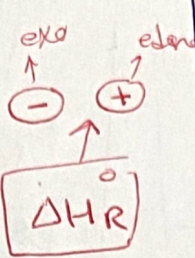
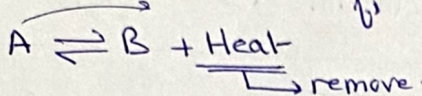
بالإضافة إلى

بالإضافة إلى

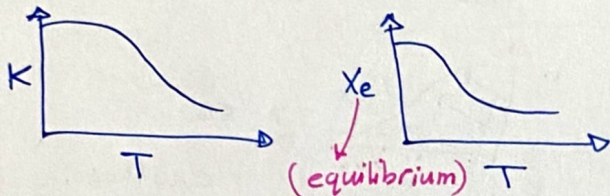
Nonisothermal Reactor Design Adiabatic Equilibrium Conversion

X equilibrium conversion

$X_e \rightarrow$ endothermic.
 $X_e \rightarrow$ exothermic



Exothermic Reaction

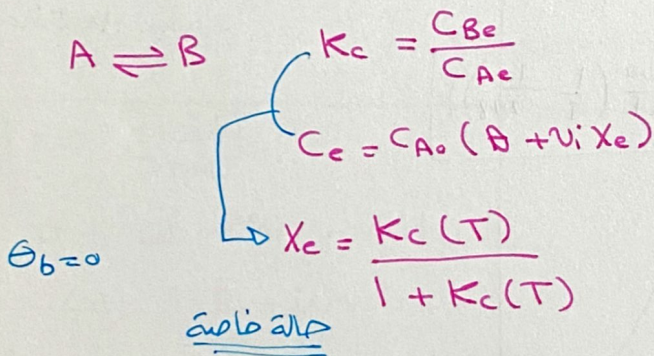


$\downarrow K \uparrow T$
product

product
 $X_e \downarrow$
 $T \uparrow$

* Adiabatic Temperature & Adiabatic Equilibrium Conversion

equilibrium constant X_e stoichiometry



Temp function $\leftarrow K_c$

Energy balance.

$$F_{A0} \sum \theta_i C_{pi} (T - T_0) + (F_{A0} X) [\Delta H_{rxm}(T) + \Delta C_p (T - T_R)] = \dot{Q} - \dot{W}_s$$

$$T = \frac{-\Delta H(T_R) X + \sum \theta_i C_{pi} T_0 + X \Delta C_p T_R}{\sum \theta_i C_{pi} + X \Delta C_p}$$

$$X = \frac{\sum \theta_i C_{pi} (T - T_0)}{-\Delta H_{rxm}(T_R) + \Delta C_p (T - T_R)}$$

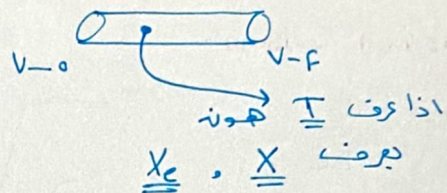
$$X_e = \frac{K_c(T_e)}{1 + K_c(T_e)}$$

$$X_e = \frac{\sum \theta_i C_{pi} (T_e - T_0)}{-\Delta H_{rxm}(T_R) + \Delta C_p (T_e - T_R)}$$

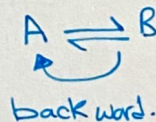
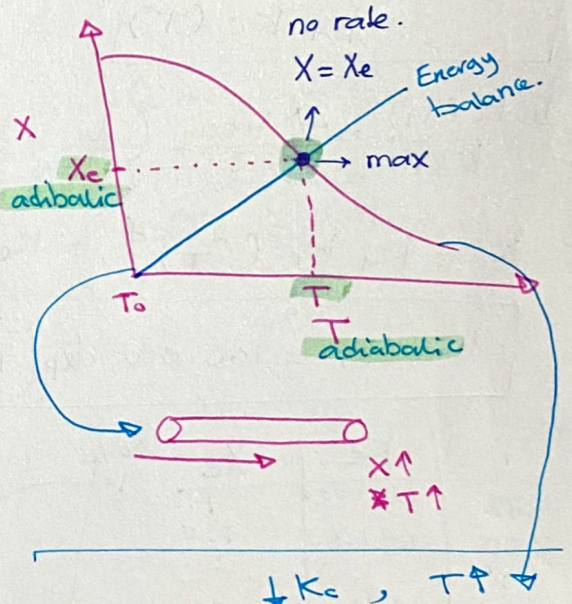
(function Temp)

reactor T بال

و يعرف X_e , X و موقع



!?! X maximum



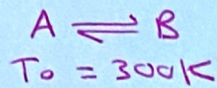
$$X_e \downarrow = \frac{K_c \downarrow}{1 + K_c \downarrow}$$

adiabatic T
adiabatic X_e

rate

بساوي اعلاي و بطرح T_e
اومدة الر

Example:-



$$T_0 = 300K$$

Plot =? $X_e \rightarrow$ function T

$$K_e = 100\,000 \text{ at } 298K$$

ΔH_f	A	B
	-40 000	-60 000
C_p	50	50

Solution

$$\Delta C_p = 0, \Delta H_{rxn} = -20\,000$$

↓
exothermic

→ Equilibrium Constant

$$K_c = \frac{C_{Be}}{C_{Ae}}$$

$$C_{ie} = C_{A0} (\theta_i + \nu_i X_e)$$

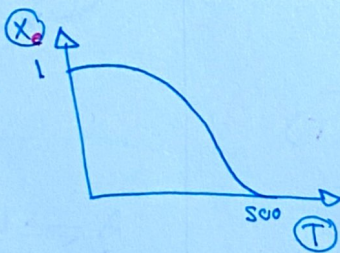
$$X_e = \frac{K_c (T)}{1 + K_c (T)}$$

$$\ln \frac{K(T_2)}{K(T_1)} = -\frac{\Delta H_{rxn}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

$$K = K_y K_c (C_T)^{-\delta} = K_c$$

$$K_c(T) = 100\,000 \exp \left(\frac{-20000}{1.987} \left(\frac{1}{T} - \frac{1}{298} \right) \right)$$

T	K_c	X_e
298	100 000	1.0
350	661.60	1.0
...	...	...
500	0.12	0.11



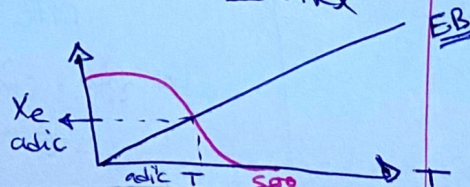
→ Energy balance

(X at function Temp.)

$$F_{A0} \sum C_p (T - T_0) + (F_{A0} X) (\Delta H_{rxn}(T_e) + \Delta C_p (T - T_e)) = 0$$

$$X_{EB} = \frac{\sum \theta C_p (T - T_0)}{-\Delta H_{rxn}} = \frac{C_p (T - T_0)}{-\Delta H_{rxn}}$$

T	X_{EB}
300	0
400	0.25
500	0.75

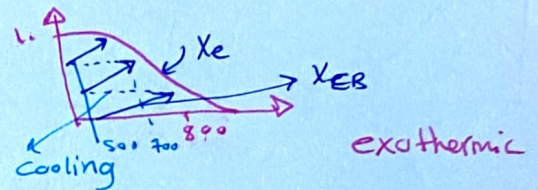
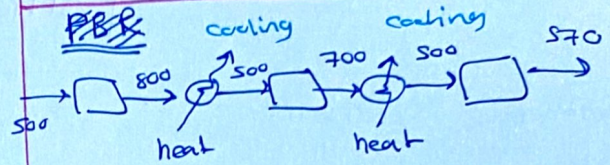


as the 465K = T_e (adiabatic temp)
0.42 = X_e

$$X_e = \frac{K_c(T)}{1 + K_c(T)}$$

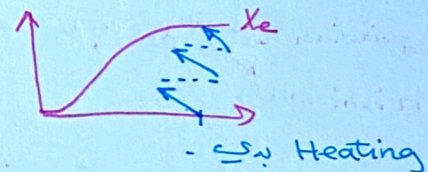
$$X_{EB} = \frac{C_p (T - T_0)}{-\Delta H_{rxn}}$$

maximum J_1, P, L, Q



equilibrium is not possible at this rate

indothermic



CSTR with Heat effect.

well mixed + T uniform
isothermally $\Delta T = 0$

* isothermal $\rightarrow$ feed Temp
identical of the fluid
inside CSTR

$$(T = T_0)$$

constant T $\rightarrow$ $\Delta T = 0$
energy balance

Heat Q $\rightarrow$ $\leftarrow$ $\rightarrow$ $\leftarrow$
remove heat

T or Q $\rightarrow$ $\leftarrow$ $\rightarrow$ $\leftarrow$

EB $\rightarrow$ (T, V, X) *

(two equation) $\rightarrow$ design
Energy
 X T

EB $\rightarrow$ steady
state

$$0 = \dot{Q} - \dot{W}_s - \Delta H$$

$$\Delta H = \dot{Q} - \dot{W}_s$$

$$F_{A0} \sum \theta C_p (T - T_0) + (F_{A0} X) \Delta H_{rxn}(T) = \dot{Q} - \dot{W}_s$$

$$F_{A0} X = \text{input}$$

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

$$F_{A0} \sum \theta C_p (T - T_0) + (-r_A) V \Delta H_{rxn}(T) = \dot{Q} - \dot{W}_s$$

combine Energy balance.

$$F_{A0} \sum \theta C_p (T - T_0) + (F_{A0} X) \Delta H_{rxn}(T) = \dot{Q} - \dot{W}_s$$

given X

neg. $\dot{W}_s$

$\dot{Q} = ? \rightarrow$ heat
reactor $\rightarrow$ (should be removed)

$$\dot{Q} = ?$$

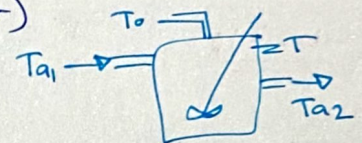
(coolant)

$$\dot{Q} = \dot{m}_c C_{p,c} (T_{a2} - T_{a1})$$

$$\dot{Q} = UA \Delta T_{Lm}$$

$$\dot{Q} = \frac{UA (T_{a1} - T_{a2})}{\ln \left[\frac{(T_{a1} - T)}{(T_{a2} - T)} \right]}$$

transferred
from reactor



* In high coolant flow rate
($T_{a2} \approx T_{a1} = T_a$)

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

$\dot{m}_c = ?$ ΔT_c
($T_{a2} - T_{a1}$)

$$\Delta H = \dot{Q} - \dot{W}_s$$

$$\dot{Q}_c = \dot{m}_c C_{p,c} (T_{a2} - T_{a1})$$

$$T_{a2} = ?$$

$\dot{m}_c$ T_{a1} $\rightarrow$ specified

$$\dot{Q}_{reactor} = \dot{Q}_{coolant}$$

$$T_{a2} = T - (T - T_{a1}) \exp \left(\frac{-UA}{\dot{m}_c C_{p,c}} \right)$$

Case 1: X specified
calculate $\rightarrow T \& V$?

$X \xrightarrow[\text{EB}]{\text{calculate}} T$

$T \xrightarrow[\text{Arh.}]{\text{calculate}} K$

$K, X \xrightarrow{\text{calculate}} r_A$

$r_A, X \xrightarrow[\text{M.B.}]{\text{calculate}} V$

Case 2: T specified
calculate $\rightarrow X \& V$?

$T \xrightarrow[\text{EB}]{\text{calculate}} X$

$T \xrightarrow[\text{Arh}]{\text{calculate}} K$

$K, X \xrightarrow{\text{calculate}} r_A$

$r_A, X \xrightarrow[\text{M.B.}]{\text{calculate}} V$

Case 3: V specified
calculate $\rightarrow X \& T$?

Solve EB + MB Equation

Simultaneous calculation

$X_{MB} = f(T) \& X_{EB} = f(T)$

$T \& X$

* بالعوض از ب
خطوط اعداد
و فترت بالا بال اعداد

Example: $A + B \rightarrow C$

$A + B \rightarrow C$

$V_{0A1} = 46.62$

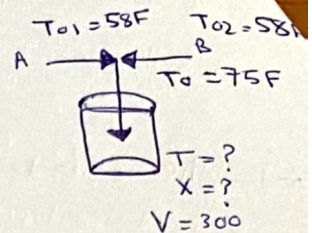
$F_{A01} = 43.04$

$F_{A01} = 71.87$

$V_{M01} = 46.62$

$F_{I102} = 802.8$

$V_{I102} = 233.1$



$H_0^t < H_{01}^t + H_{02}^t$
(58F) (58F)
75

Assume

$V_0 = V_A + V_{M01} + V_{B02}$

V_0 is 3% less

$K = A e^{-E/RT}$
 $K = 16.96 \times 10^{12} \times e^{-32.4/RT}$

$E = L$

ΔH	MCH	PO	H2O	PG
CP	-	-	-	-

X, T unknown $T = 125F$
(Should not exceed)

$V = \frac{F_{A0} X}{-r_A}$ $X_{MB} \rightarrow$ Function (T)

$X_{MB} = \frac{TK}{1+TK}$ $\rightarrow$ بالعوض از ب

عوضنا بدين ..

Energy Balance

$F_{A0} \sum \Theta C_p (T - T_0) + F_{A0} X \Delta H_{Rx}(T) =$

$\frac{F_{A0} X}{V} \Delta H_{Rx}(T) =$

$X_{EB} = \frac{\sum \Theta C_p (T - T_0)}{[\Delta H_{Rx}(T_f) + \Delta C_p (T - T_f)]}$

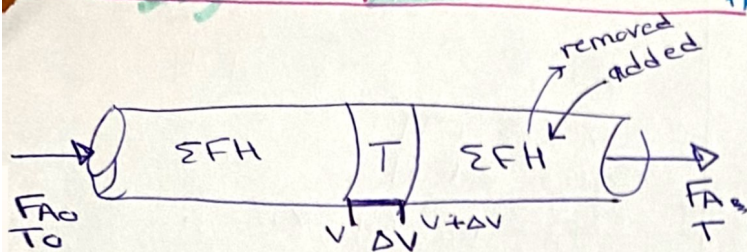
عوضنا بدين ..

و اعداد بدين T اعداد

T	X_{MB}	X_{EB}
-	-	-
-	-	-
-	-	-

في امانة
بالعوض بدين

Heat transfer in non-isothermal (PFR)



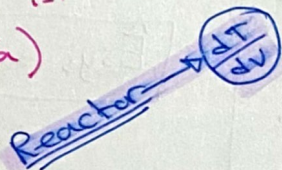
$$\Delta \dot{Q} = U \Delta A (T_a - T) \\ = U a (T_a - T) \Delta V$$

ليجول
 $\Delta \dot{Q} = q'' dA$

Energy balance

$$\sum F_i H_i - \sum F_i H_i + \Delta \dot{Q} = 0$$

$$\frac{dT}{dV} = \frac{U a (T_a - T) + [-\Delta H_{rx}(T_r) - \int_{T_r}^T \Delta C_p dT] - r_A}{F_{A0} (\sum_{i=1}^n \theta_i C_{pi} + X \Delta C_p)} - r_A \\ = F(X, T, T_a)$$



$$\frac{dT}{dV} = \frac{r_A \Delta H_{rx} - U a (T - T_a)}{\sum F_i C_{pi}}$$

PFR (X) = S_v

$$\frac{dT}{dV} = \frac{r_A \Delta H_{rx} - U a (T - T_a)}{F_{A0} (\sum \theta C_p + \Delta C_p X)}$$

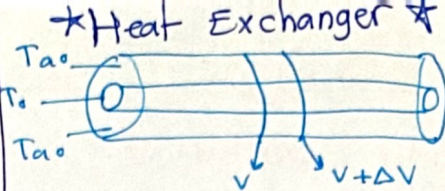
PBR (X) = S_v

$W = F_b V$

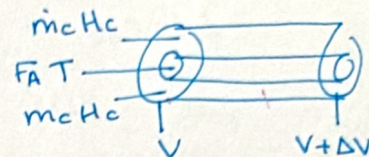
$$\frac{dT}{dW} = \frac{r_A' \Delta H_{rx} - \frac{U a}{F_b} (T - T_a)}{\sum F_i C_{pi}}$$

$$\frac{dT}{dW} = \frac{r_A' \Delta H_{rx} - \frac{U a}{F_b} (T - T_a)}{F_{A0} (\sum \theta_i C_{pi} + \Delta C_p X)}$$

$a = \frac{A_s}{V}$



Co - Current Flow



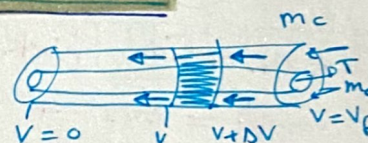
$$mC H_c - mC H_c + U a (T - T_a) \Delta V = -mC \frac{dH_c}{dV} + U a (T - T_a) = 0$$

$$\frac{dH_c}{dV} = C_{pc} \frac{dT_a}{dV}$$

$$\frac{dT_a}{dV} = \frac{U a (T - T_a)}{mC C_p} = f(T, T_a)$$

At V=0
 $T_a = T_{a0}$

Counter Current Flow



$$mC \frac{dH_c}{dV} + U a (T - T_a) = 0$$

$$\frac{dT_a}{dV} = \frac{U a (T_a - T)}{mC C_p}$$

At V=0
 $T_a = T_{a2} = ?$

- 1) Mole Balance initial condition
- 2) Rate Law
- 3) Stoichiometry
- 4) Energy Balance

Reactor $\frac{dT}{dV}$

Co-current Counter current $\frac{dT_a}{dV}$

rate $K = A e^{-E/RT}$ = ③

Ch15

* Energy Balance

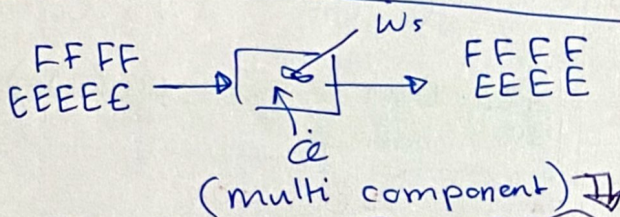
endo, exothermic.

كل تفاعل يحدث يا بمتغيريا يعطي حرارة.
قيمة الحرارة بتعطي وتحدد P و T و نوع المادة.
دفعته نحسبها ΔH_{Rxn}

$$\text{Rate heat} - \text{Rate work} + \text{added} - \text{leaving} = \text{accumulation}$$

$$\dot{Q} - \dot{W} + \sum F_{in} E_{in} - \sum F_{out} E_{out} = \frac{d\hat{E}}{dt}$$

المعادلة العامة لحفظ الطاقة (معادلة الاصل)



$$\dot{Q} - \dot{W} + \sum F_{in} E_{in} - \sum F_{out} E_{out} = \frac{d\hat{E}}{dt}$$

Evaluation Work (W) = ?

$$\dot{W} = \dot{W}_s + \text{Rate of flow Work}$$

$$\text{Rate of flow Work} = - \sum F P \hat{V}|_{in} + \sum F P \hat{V}|_{out}$$

(Pressure Volume)

Evaluation Energy (E) = ?

$$E_i = U_i + \frac{1}{2} m v^2 + m g z$$

$$E_i \approx U_i$$

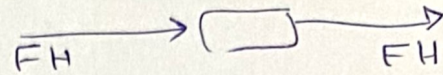
internal energy

multiple component معادلة enthalpy

$$H = U + PV$$

$$\dot{Q} - \dot{W}_s + \sum F H|_{in} - \sum F H|_{out} = \frac{d\hat{E}}{dt}$$

exo ←
endo ←



$$I_n = \sum F H$$

$$out = \sum F H$$

$$F_A = F_{A0} (1 - x)$$

$$F_B = F_{A0} (\theta_B - \frac{b}{a} x)$$

Energy Conversion

$$\dot{Q} - \dot{W}_s - F_{A0} \left[\sum \int \theta C_p dT \right] - F_{A0} x \Delta H = \frac{d\hat{E}}{dt}$$

$$\hat{E}_{sys} = \sum N E_i$$

$$= \sum N U_i$$

$$= \sum N (H - PV)$$

$$= \sum N H - P \sum N V$$

neglect
نسيء

$$\hat{E}_{sys} = \sum N H$$

...
نسيء

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum F_{A0} (H - H_{id}) + (-\Delta H_{Rx}) (-r_A V)}{\sum N_i C_{p,i}}$$

CSTR, semibatch

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum F C_p (T - T_{id}) + (-\Delta H_{Rx}(T)) (-r_A V)}{\sum N_i C_p}$$

(liquid case)

$C_p \rightarrow$ neglect

$$\sum N C_p = N_{A0} C_{p,i}$$

$$\sum F C_p = F_{A0} C_{p,e}$$

Energy Balance on Batch Reactor (BRs)

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - F_{A0} C_p (T - T_0) + (-\Delta H_{RX}^* - r_A V)}{N_{A0} C_p}$$

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s + (-\Delta H_{RX}^* - r_A V)}{\sum N_i C_{p,i}}$$

(Steady state)

(unsteady state)

$$\frac{dT}{dt} = \frac{\dot{Q}_{gb} - \dot{Q}_{rb}}{N_{A0} (\sum \theta C_p + \Delta C_p X)}$$

$$\dot{Q}_{gb} = -\Delta H_{RX}^* - r_A V$$

$$\dot{Q}_{rb} = \dot{m} C_{p,c} (T - T_{ai}) \left(1 - \exp\left(\frac{-UA}{\dot{m} C_p}\right) \right)$$

$$T_{a2} = T - (T - T_{ai}) \left(1 - \exp\left(\frac{-UA}{\dot{m} C_p}\right) \right)$$

Case 1 Adiabatic + unsteady state
(Batch)

$$X = \frac{\sum \theta C_p (T - T_0)}{-\Delta H_{RX}}$$

$$T = T_0 + \frac{-\Delta H_{RX} X}{\sum \theta C_p + X \Delta C_p}$$

Case 2 Heat Exchanger Batch

$$\frac{dT}{dt} = \frac{\dot{Q}_g - \dot{Q}_r}{N_{A0} C_p}$$

$$\dot{Q}_r = \dot{m} C_p [(T - T_{ai}) \left(1 - \exp\left(\frac{-UA}{\dot{m} C_p}\right) \right)]$$

$$\dot{Q}_g = (-r_A V) (-\Delta H_{EX})$$

$$-r_A V = N_{A0} K (1 - X)$$

Example

$$C_{p0} = \sum \theta C_p$$

1) Mole Balance.

2) Rate law

3) Stoichiometry $\Rightarrow N_A = N_{A0} (1 - X)$

4) Energy balance.

F_{A0} is Batch

* Unsteady state semi batch Reactor: -

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum F_{Ai} C_{p,i} (T - T_0) - (-\Delta H_{RX}^*)}{\sum N_i C_{p,i}}$$

$$\frac{dT}{dt} = \frac{\dot{Q}_{gs} - \dot{Q}_{rs}}{\sum N_i C_{p,i}}$$

$$\dot{Q}_{gs} = r_A V \Delta H_{EX}$$

$$\dot{Q}_{rs} = \sum F_{i0} C_{p,i} (T - T_0) + \dot{m} C_{p,c} (T - T_0) \left(1 - \exp\left(\frac{-UA}{\dot{m} C_p}\right) \right)$$

Example

Energy Balance

Collection and analysis of Rate Data

In this class we will study the determination rate order and constant using:

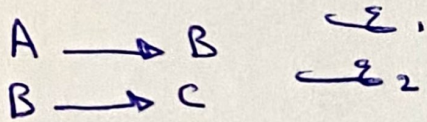
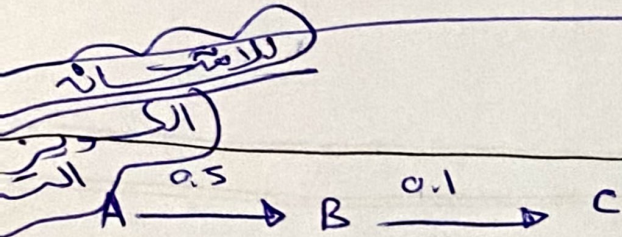
1. Method of Excess (initial rate method)
2. Method of half-lives
3. Integral Method
4. Differential Method

سنوات

$$\sum_{j=1}^m N_{j0} C_{pj}$$

For large coolant
flow rates

$$\frac{dT}{dt} = \frac{V \sum_{i=1}^q r_{ij} \Delta H_{Rxi} - UA(T - T_a) - \sum_{j=1}^m F_{j0} C_{pj} (T - T_0)}{\sum_{j=1}^m N_j C_{pj}}$$



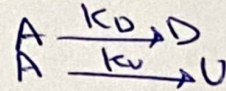
$$\begin{aligned} C_A &= C_{A0} - \epsilon_1 \\ C_B &= C_{B0} + \epsilon_1 - \epsilon_2 \\ C_C &= +\epsilon_2 \end{aligned}$$

$$\epsilon_1 = C_{A0} - C_A = 10 - 4 = 6$$

$$S = 5 = \frac{\epsilon_1}{\epsilon_2} \Rightarrow \epsilon_2 = \frac{\epsilon_1}{5} = \frac{6}{5} = 1.2$$

$$C_D = 6 - 1.2 = 4.8$$

$$y = \frac{C_B}{C_{A0} - C_A}$$



$$S_{DU} = 1 = \frac{-r_D}{r_U} = \frac{K_D C_A}{K_U C_A} = \frac{0.1}{0.1}$$

$$\begin{aligned} C_A &= C_{A0} - \epsilon_1 - \epsilon_2 \\ &= C_{A0} - 2\epsilon \end{aligned}$$

$$\epsilon_1 = \frac{C_{A0} - C_A}{2} = \frac{10 - 1.3}{2} = 4.32$$

$$\begin{aligned} C_D &= C_{D0} + \epsilon_1 \\ C_D &= 4.32 \end{aligned}$$

...line with a slope of 1.0.
 ...ould yield a straight line with a slope of 2.0.

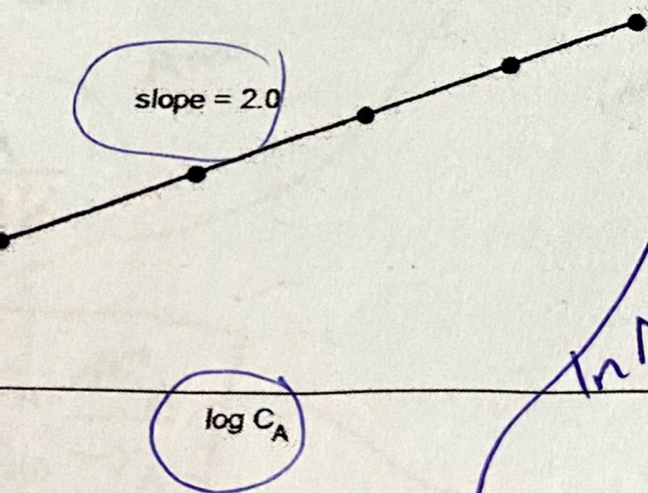
$\log r = -2.76 + 2.0 \log C_A$
 the data suggest a slope of 2!

$$\log k_2 = -2.76$$

$$k_2 = 1.73 \times 10^{-3} \text{ L/mol s}$$

$\log C_A$
 slope of 2!

Is



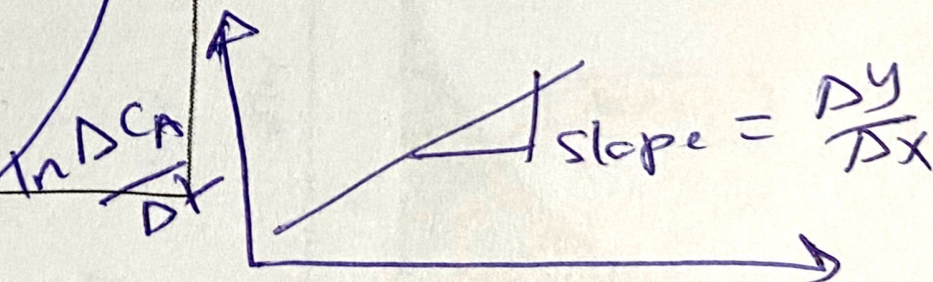
معدل التفاعل

t/P	$C_P = \frac{PV}{RT}$	$\ln C$	$\frac{\Delta C}{\Delta t}$	$\ln \frac{\Delta C}{\Delta t}$
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$$\frac{dC_A}{dt} = r = K C_A^n$$

$$\left| \frac{\Delta C_A}{\Delta t} \right| = K C_A^n$$

$$\ln \left| \frac{\Delta C_A}{\Delta t} \right| = \ln K + n \ln C_A$$



$$\ln C_A$$

$$E = \ln K$$

$$K = e^E$$