

Chemical Engineering

Industrial Chemical

Reaction Engg.

L1

Industrial Process

(Sandi ma'am's part)

Chemical Rxn Engg \rightarrow used in Industries where Chemical Processes take place.

Reactants \rightarrow Products.



Even if $\Delta r G < 0$ the Rxn may not proceed due to :-

(1) Rate of Rxn is very less (very less molecules undergo rxn - which is negligible)

(2) Ea is very high.

Process with high Ea requirement ($k = A e^{-E_a/RT}$) has less rate

process

Thermodynamics

\rightarrow tells us the Possibility of Rxn

Kinetics

\rightarrow tells whether rxn proceeds or not

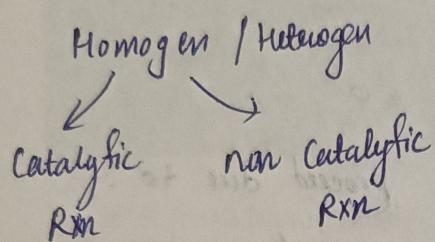
Reaction Coordinate :- Energy profile Change with time
between Reactants - Intermediate products /
Transition state - Products.

Reaction Coordinate :- Change in Energy w.r.t change in bond angle / bond length during progress of the rxn.

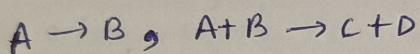
Thermodynamics :- generally does not include time

Homogeneous Reactions

1. Reactions involving molecules of same phase
2. Gas phase Rxn.



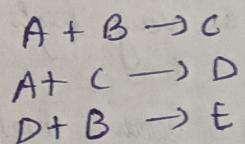
Single Rxn



Heterogeneous Reactions

1. Reactions Involving molecules of different phases
2. Solid-gas, solid-liquid, solid-gas-liquid rxn

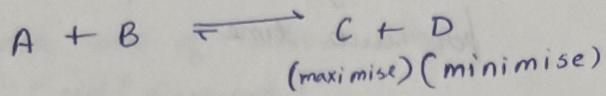
Multiple Rxns (Side Rxns)



Order & Molecularity,
Elementary & Non Elementary

Physical
adsorpt
vander waals

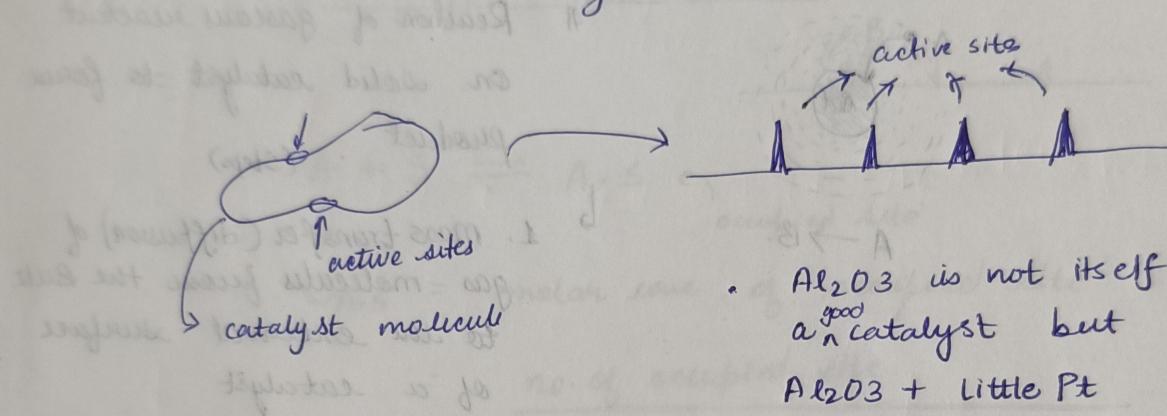
(sonali ma'am's
part)



$$\text{selectivity} = \frac{n_C \text{ formed}}{n_D \text{ formed}}$$

(*) With time the activity of a catalyst decreases.

↳ called Catalyst Deactivation

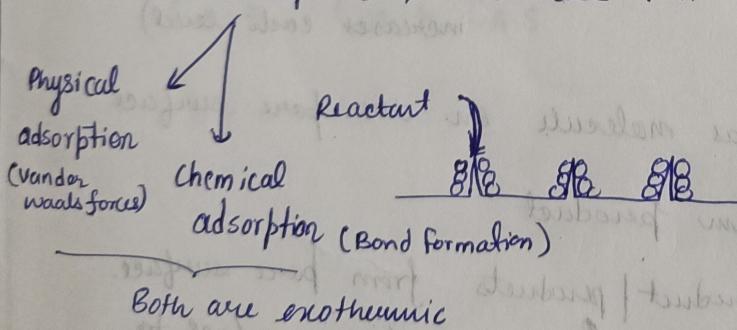


- Al_2O_3 is not itself a good catalyst but $\text{Al}_2\text{O}_3 + \text{Little Pt}$

is a highly active catalyst

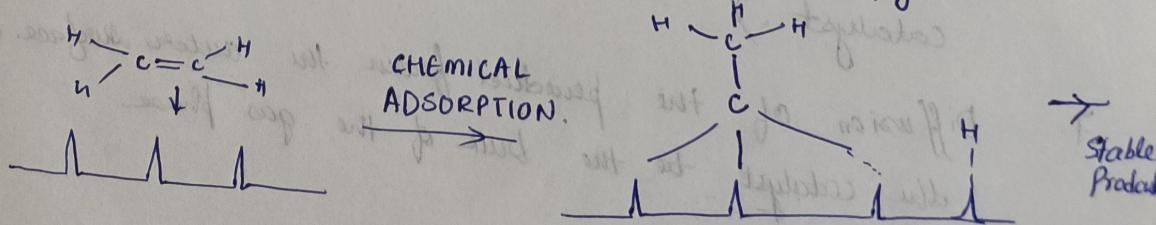
- These Pt sites are the active sites.

- From Adsorption, chemical rxn starts



ΔH in Physical adsorption = 1 - 15 kcal/g mol.

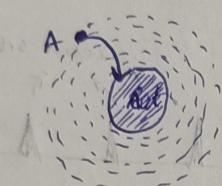
ΔH in Chemical adsorption = 10 - 100 kcal/g mol.



(Turnover frequency (N)):- No. of atoms/ molecule/ complex reacts on the catalyst surface per active site per unit time.

Dispersion (D) for a supported catalyst = % of active metals dispersed on the catalyst per unit area.

Gas Phase - Solid Catalytic Reaction :-



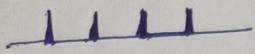
Reaction of gaseous reactant on solid catalyst to form product (steps)

b) 1. Mass transfer (diffusion) of gas molecules from the bulk to the external surface of a catalyst

2. Mass transfer of gas molecule from the external surface to the pore surface.

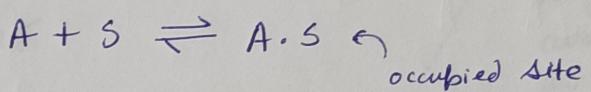
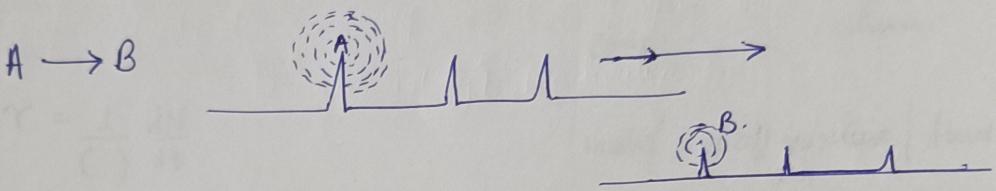
(as resistance to diffusion increases each level)

3. Adsorption of the gas molecule on the pore surface
4. Reaction to form product
5. Desorption of product/ products from pore surface.
6. Diffusion of product from the pore surface to the pore mouth or (external surface of the catalyst.)
7. Diffusion of the product from the outer surface of the catalyst to the bulk of the gas phase



C_A = molar conc. of active sites
(mol/g catalyst)

$$= \frac{\text{no. of total active sites}}{\text{g of catalyst} \times \text{Avogadro number}} = \text{molar conc. of active sites.}$$



$$C_{A \cdot S} = \text{molar conc. of occupied site}$$

$$= \frac{\text{no. of occupied site}}{\text{g. of catalyst} \times \text{Avogadro number}}$$

$$C_V \text{ (vacant site)} = \frac{\text{no. of vacant site}}{\text{g. of catalyst} \times \text{Avogadro no.}}$$

Site Balance

$$C_A = C_V + C_{A \cdot S}$$

L-2
(Part by Koushuv Sir)

(*) Specific Rate Constant \underline{k} ←
Reaction rate Constant = k
reaction velocity constant = k

remember, it is small k .

Batch Reactor Data.

conc time

mole / vol of mixture / time
or

Surface of
catalyst
or

weight of catalyst

for Heterogeneous
rxn.

For Homogeneous
Rxn.

$$(-r_A) = k c_A$$

a function of temperature

Arrhenius Eqⁿ

$$k = A e^{-E_a/RT}$$



It is for Elementary Rxn.

For non-elementary step:- We use this eqn but with

$$E_a = E_{a, RDS}$$

($\leq 10\%$ error)

A is called frequency factor.

↳ mild dependency on temperature

↳ considerable dependency on pressure.

Jane Smith Exp - 2.3

Run	t (min)	Conv (%)	Cone. (outlet)
1	13	11.2	$0.1(1 - 0.112) = 0.1176/2 = 0.0588$
2	34	26.7	$0.1(1 - 0.257) = 0.1486/2 = 0.074$
3	59	36.7	$0.1(1 - 0.367) = 0.1266 = 0.063$
4	120	55.2	$0.1(1 - 0.552) = 0.0896 = 0.0447$

$$C_0 = 0.2 \text{ molal}$$

$$X = 1 - \frac{C_{\text{out}}}{C_0} = 1 - \frac{C}{C_0}$$

$$1-X = \frac{C}{C_0}$$

$$C = C_0(1-X)$$

1st order reaction rate \rightarrow

$$\dot{A} = -\frac{d[A]}{dt} = k_1 [A] \rightarrow \ln \left[\frac{[A]_0}{[A]} \right] = k_1 t$$

2nd order Reaction Rate

$$\dot{A} = -\frac{d[A]}{dt} = k_2 [A][B] \rightarrow k_2 t = \frac{1}{[A]_0} - \frac{1}{[A]}$$

$$\therefore \text{at } t=0, [A]_0 = [B]_0 = 0.1$$

$$\therefore x = \frac{[A]_0 - [A]}{[A]_0}$$

$$[A] = [A]_0(1-x)$$

$$= 0.1(1 - 0.112) = 0.1 \times 0.888$$

$$= 0.0888$$

k_1

1.5

3.80

5.8

1.02

k_2

Fogler
Book

$$k_1 = \frac{1}{t} \ln\left(\frac{C_{AO}}{C_A}\right)$$

$$\begin{array}{c|c} k_1 & \\ \hline 1.52286 \times 10^{-4} & \\ 3.808 \times 10^{-4} & 1.456 \times 10^{-4} \\ 5.86 \times 10^{-4} & 1.2917 \times 10^{-4} \\ 1.029 \times 10^{-3} & 1.115 \times 10^{-4} \end{array}$$

$$\begin{array}{c|c} k_2 & \\ \hline 1.617 \times 10^{-3} & \\ 1.69 \times 10^{-3} & \\ 1.637 \times 10^{-3} & \\ 1.71 \times 10^{-3} & \end{array}$$

$$\text{Avg} = 1.67 \times 10^{-3}$$

$$\begin{aligned} k_2 &= \frac{1}{t} \left[\frac{1}{C_A} - \frac{1}{C_{AO}} \right] \\ &= \frac{1}{t} \cdot \left[\frac{1}{C_{AO}(1-x)} - \frac{1}{C_{AO}} \right] \\ &= \frac{\frac{1}{1-x} - 1}{\frac{1}{1-x}} = \frac{x}{1-x} \\ &= \frac{1}{t C_{AO}} \cdot \frac{x}{1-x} \end{aligned}$$

\therefore Isothermal conditions are maintained, k must remain constant & k_2 data is more convincing

Why differential method is better than the Integral method?

↓
Shows data points & intermediate data points more clearly.

Integral method masks the intermediate set of points

$$\left[\frac{1}{(x_A)} - \frac{1}{A_0} \right] \cdot \frac{1}{t} = \dots$$

$$\left(\frac{1}{x_A} - \frac{1}{(x-1)x_A} \right) \cdot \frac{1}{t}$$

$$\left[1 - \frac{1}{x-1} \right] \cdot \frac{1}{(x_A)t}$$

$$= \frac{x}{x-1} - 1$$

$$\frac{x}{x-1} = \frac{1}{(x_A)t}$$

second term is decreasing
characteristics mean this is additional
is work of dominant effect
is work of disturbance

Reactor Design

Inherent characteristics

Kinetic

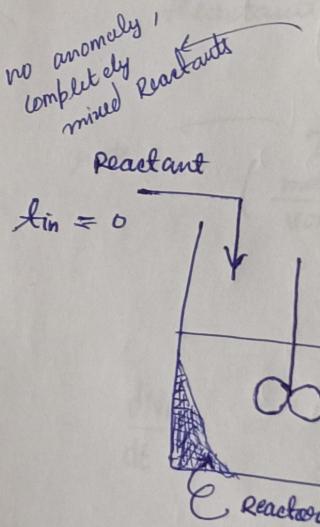
mechanism

Rate Law

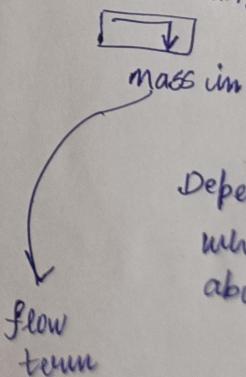
Activation Energy



not input conditions
but are
for the design



Continuity Eqn



Depending upon
whether we
absent Re

Reactor Design -

Inherent characteristics of Rxn

Kinetics

mechanism

Rate Law

Activation Energy

not input conditions
but are important
for the designing.

7 Feb
Class Test

Design

Input Conditions

Calculate
and
check / verify.

* keep in mind the standards

Ex: SS 316 is a standard Stainless Steel material for design.

* Temperature

* Pressure

* Mass flow Rate

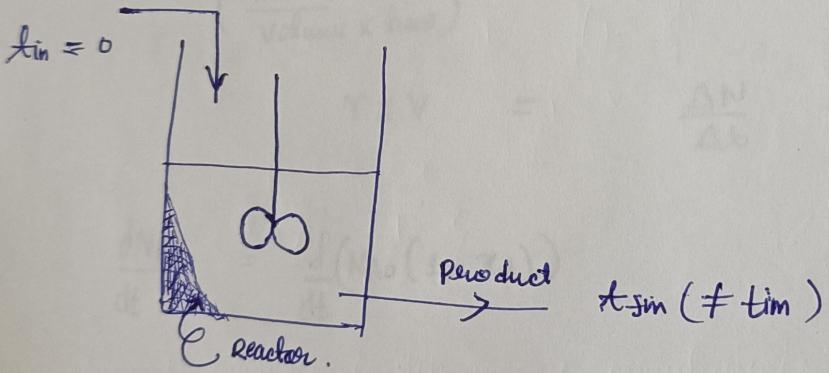
* Enthalpy - ΔH / Heat Effects.

* mixing characteristics

no anomaly,
completely
mixed Reactants

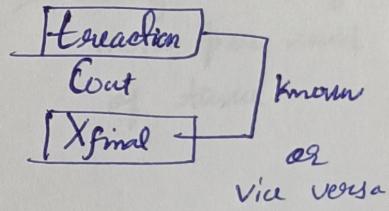
Ideal

Batch Reactor
Design



Pharmaceuticals
use it. cost
considerations.

$V_{batch} \rightarrow *$



Continuity Eqn | Mass Balance Eqn



mass in

$$-\text{mass out} + \text{mass generated} = \text{mass accumulated.}$$

\downarrow \uparrow

Depending upon

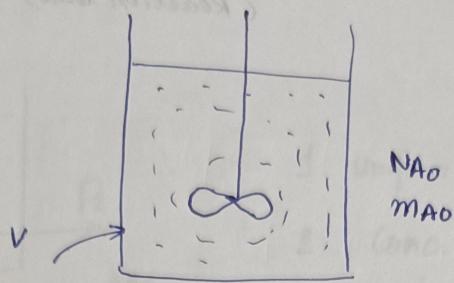
whether we are talking
about Reactant or Product

flow term

Book
beloved

Batch

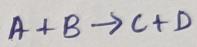
Conservation law:



Assumption:-

1. Uniform through mixing.

$r_{in} t_{in}$ \rightarrow accumulation.



* Write Design Eqn w.r.t to the limiting Reactant.

$$\text{rate} \leftarrow r \times V \times \Delta t = \Delta N$$

$\left(\frac{\text{moles}}{\text{volume} \times \text{time}} \right)$

$$r \times V = \frac{\Delta N}{\Delta t} \Rightarrow \text{change in no. of moles per unit of time}$$

$$\frac{dN_A}{dt} = \frac{d}{dt}(N_{A0}(1-x_A))$$

$$= -N_{A0} \frac{dx_A}{dt} = -rV$$

$$\int_{x_A=0}^{x_A} \frac{dx_A}{-rV} = - \int_{t=0}^t \frac{dt}{N_{A0}}$$

$$N_{A0} \cdot \int_0^{x_A} \frac{dx_A}{(-rV)} = \int_0^t dt$$

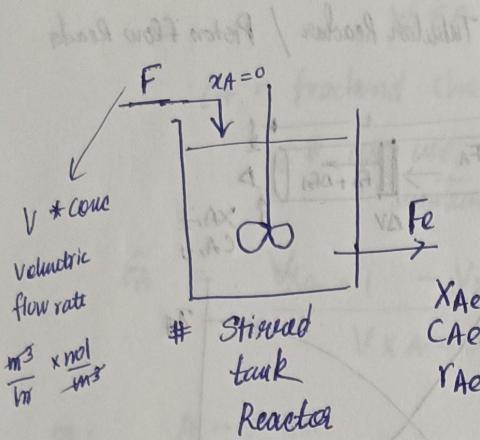
If volume varies

$$V = V_0 (1 + \epsilon_A x_A) = V_0 (1 + \epsilon_B x_B)$$

$$x_A \epsilon_A = x_B \epsilon_B$$

[fractional change x conversion]

CSTR $\xrightarrow{\text{continuous flow}}$ PFR



1. Uniform Stirring

2. Conc. inside the reactor is always constant.

3. Flow Rate Remains Constant.

4. * Inside this Reactor, one constant rxn rate irrespective of time. (Isothermal conditions needed)

mass in - mass out \pm mass generated = mass accumulated

$$F_A(1-x_i)\Delta t - F(1-x_e)\Delta t - rV \Delta t = 0 \quad (\because \text{flow Reactor})$$

$$\frac{V}{F} = \frac{X_{A,e}}{(-r_A)}$$

$$\frac{V}{F} = \frac{V_i}{V_{CAO}} = \frac{T}{CA_0}$$

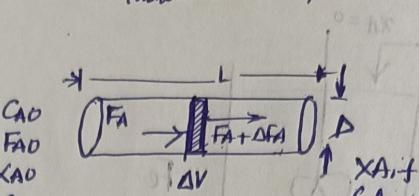
↓
volumetric flow rate \times conc

$$T = \frac{CA_0 \cdot X_{Ae}}{(-r_A)}$$

Continuous steady state Plug Flow Reactor.

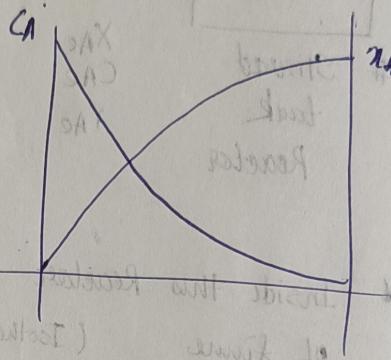
$$V = V_0 (1 + \epsilon x)$$

Tubular Reactor / Piston flow Reactor



$$\frac{dF}{dV} = (-r_A)$$

$$\left(+ F_{A0} \right) \frac{dx_A}{dV} = (-r_A)$$



$$\int_0^V \frac{dV}{dV} = V = F_{A0} \int_0^{x_A} \frac{dx}{(-r_A)}$$

$$\frac{V}{F_{A0}} = \frac{V}{C_{A0}} = \int_0^{x_A} \frac{dx}{(-r_A)}$$

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

irrespective of shape.

Volumetric feed rate

Constant Density Reactor

$\frac{x_A X}{(1 - X)}$ use X rather than conversion

if V changes

it can change due to change in moles

$$V = V_0 (1 + \epsilon x)$$

$$\frac{\delta A X - \delta A}{(1 - X)}$$

$$\epsilon = \delta X Y_{AO}$$

$$\delta = \frac{1 + \epsilon}{1 - \epsilon} - \frac{1}{\epsilon} - 1$$

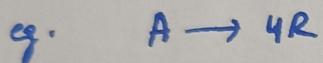
$$V = V_0 (1 + \epsilon_A X_A) , \quad X_A = \frac{V - V_0}{V_0 \epsilon_A}$$

$$\text{or } dX_A = \frac{dV}{V_0 \epsilon_A}$$

ϵ_A = fractional change in volume of the system b/w i & A
 (* We use this when the reactor Volume is not constant)

$$\epsilon_A = \frac{V_{XA=1} - V_{XA=0}}{V_{XA=0}}$$

X_A = fractional conversion of A



$$\text{Starting with pure A : } \epsilon_A = \frac{4 - 1}{1} = 3$$

$$N_A = N_{AO} (1 - X_A)$$

$$C_A = \frac{N_A}{V} = \frac{N_{AO}}{V_0} \cdot \frac{(1 - X_A)}{(1 + \epsilon_A X_A)} = \frac{C_{AO} (1 - X_A)}{(1 + \epsilon_A X_A)}$$

$$\frac{C_A}{C_{AO}} = \frac{1 - X_A}{1 + \epsilon_A X_A}$$

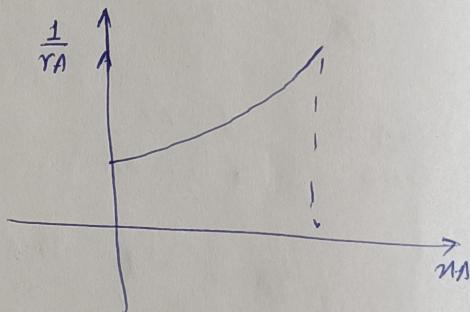
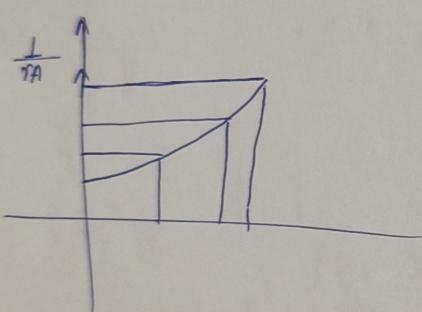
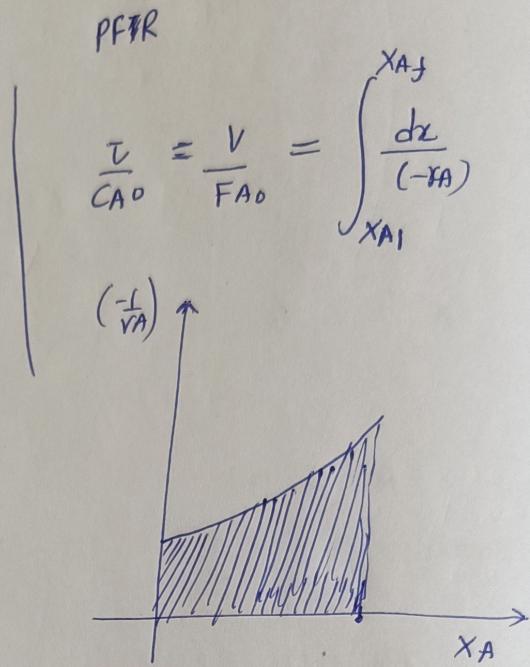
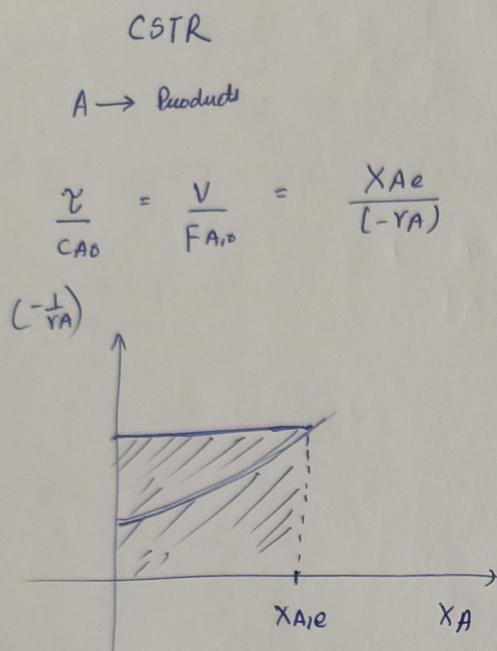
$$-r_A = -\frac{1}{V} \frac{dN_A}{dt}$$

$$-r_A = \frac{C_{AO}}{1 + \epsilon_A X_A} \cdot \frac{dX_A}{dt}$$

$$-r_A = \frac{C_{AO}}{V \epsilon_A} \cdot \frac{dV}{dt} = \frac{C_{AO}}{\epsilon_A} \cdot \frac{d(mv)}{dt}$$

Problem Solving

Ques :- A



- (*) Volume Requirement in CSTR is more than PFR
- (*) PFR is thus better in Efficiency.

$T_{PFR} =$

Single Rxn

multiple Rxn

Single Reactor

Multiple / Series of Reactor

Find T_{CSTR}

Do Again

Ques:- $A \xrightarrow{\text{Catalyst}} 3R$

$$-r_A = 10^{-2} CA^{0.5} \frac{\text{mol}}{\text{lt. sec}}$$

A goes to product with rate = r_A
so $r_A = 10^{-2} CA^{0.5}$

$CA_{1,0} = 0.0625 \text{ mol/lt}$
 $r_{1,0} = 10 \frac{\text{lt}}{\text{min}}$

Plug Flow Reactor

50 lt. A
50 lt. I
25°C
1 atm

$X_A = 0.8$

Calculate T_{PFR}

Calculate V_{PFR}

Attempt: $CA_V = \frac{F_A}{r_{1,0}}$

$$CA = \frac{CA_{1,0}}{r_{1,0}} \frac{(1 - X_A)}{(1 + \epsilon A X_A)}$$

$$CA = \frac{CA_{1,0}}{(1 + \epsilon A X_A)}$$

$$\epsilon = 8 \times \frac{V_{1,0}}{F_A}$$

$$\epsilon = (3 - 1) \times 0.5$$

$$CA_{1,0} = 0.0625 \text{ mol/lt}$$

$$T_{PFR} = \frac{(CA_0)^{1/2}}{k} \int_0^{0.8} \left(\frac{1 + X_A}{1 - X_A} \right)^{1/2} dX_A$$

$$= 33.2 \text{ sec.}$$

* * Do it.

Find $T_{CSTR} \approx 60 \text{ sec}$

Do Again if $(-r_A) = 10^2 CA$

Conclusion

$$1^{\text{st}} \text{ order } T_{CSTR} = 60 \text{ sec}$$

$$1^{\text{st}} \text{ order } T_{CSTR} = 720$$

$$2^{\text{nd}} \text{ order : } 103680$$

Any how $T_{CSTR} > T_{PFR}$

Dämköhler Number (Da)

$$Da = \frac{\text{Rate of Reaction of } A}{\text{Rate of Convective Transport of } A}$$

at initial or
 entrance condition

$$= \left(\frac{(-r_{AO}) \cdot V}{F_{AO}} \right)$$

Use of Dimensionless Numbers:-

They are used in scaling up a project to Industrial level. This parameter remains constant & we can thus scale up a laboratory setup to Industrial level setup.

$v_0 \rightarrow$ volumetric flow rate

$F_{AO} \rightarrow$ molar flow rate

$V \rightarrow$ Volume of Reactor

calculate

$$n = 1 \quad Da_{1, \text{1st order}} = \frac{(Ax - 1)}{(Ax + 1)} \cdot \frac{v_0 \cdot F_{AO}}{V} = Ax$$

$$n = 2 \text{ (notewise) right} \quad Da_{1, \text{2nd order}} = \frac{(Ax - 1)}{(Ax + 1)} \cdot \frac{v_0 \cdot F_{AO}}{V} = Ax$$

$$n^{\text{th order}} \quad Da_{n, \text{n-th order}} = \frac{(Ax - 1)}{(Ax + 1)} \cdot \frac{v_0 \cdot F_{AO}}{V} = Ax$$

$$Da = \frac{-r_{AO} \times V}{F_{AO} \left(\frac{Ax}{V} + \frac{1}{V} \right)} = \frac{(-r_{AO})}{\left(\frac{F_{AO}}{V} \right)} = k \cdot C_{AO}$$

$$C_{AO} = \frac{F_{AO}}{v_0}$$

$$\Rightarrow k \cdot \frac{V}{F_{AO}} = (Ax)$$

2nd or

n th

For 1st

DA

for CST

for PFR

axioms to DA

(ustoming)

For PFR

E

$$2^{\text{nd}} \text{ order} :- \quad Da = k C_{AO} \left(\frac{C_{AO} \cdot V}{F_{AO}} \right)$$

positioned prior to stage to proceed

$$n^{\text{th}} \text{ order} = k T C_{AO}^{n-1}$$

For 1st Order Kinetics, CSTR & PFR, write their eqns in terms of

Da

$$\text{For CSTR} : \quad \frac{T}{C_{AO}} = \frac{V}{F_{AO}} = \frac{X_{A,e}}{(-RA)}$$

(Assumption of Constant Density)

$$\frac{Da}{k \cdot C_{AO}} = \frac{X_{A,e}}{(-RA)}$$

$$(-RA) = k CA$$

for PFR

$$\frac{Da}{k C_{AO}} = \frac{X_{A,e}}{k C_{AO} (1 - X_{A,e})}$$

$$Da = \frac{X_{A,e}}{1 - X_{A,e}}$$

$$\text{For PFR} : \quad \frac{T}{C_{AO}} = \frac{V}{F_{AO}} = \int_{X_{A,i}}^{X_{A,f}} \frac{dx}{(-RA)} \quad (\text{Assumption of Constant Density})$$

$$\frac{Da}{k C_{AO}} = \int_{X_{A,i}}^{X_{A,f}} \frac{dx}{X_{A,i} k C_{AO} (1 - x)}$$

$$Da = - \ln(1-x) \Big|_{X_{A,i}}^{X_{A,f}}$$

$$Da = \ln \left(\frac{1 - X_{A,i}}{1 - X_{A,f}} \right)$$

$$Da = \ln \left(\frac{1 - x_{AO}}{1 - x_A} \right)$$

$$x_A = e^{-Da} (1 - x_{AO})$$

$$x_A = 1 - e^{-Da} (1 - x_{AO}) = 1 - e^{-Da}$$

Damkohler Number is used to calculate the Extent of Rxn,
 ↓
 property of system, depends upon entry condition

Homogeneous Liquid Phase Rxn :- $A + B \rightarrow \text{Products}$

$$V = 200 \text{ ml} \quad (-r_A) = \frac{100 \text{ lit}}{\text{mol min}} (A_C B)$$

$$v_0 = 1 \text{ lit/min}$$

$$C_{A_0} = C_{B_0} = 0.05 \text{ mol/lit}$$

$$(a) X_{PFR}?$$

$$(b) X_{CSTR}?$$

$$(c) V_{CSTR} ? \text{ if } X_{CSTR} = X_{PFR}$$

Ansatz

Soln:-

2nd Order Rxn

$$D_a = \frac{CA \times (-r_{AO}) \cdot V}{F_{AO,0}}$$

$$= \frac{100 C_{AO} C_{BO} \times V}{C_{AO} \times v_0}$$

$$= \frac{100 \times 0.05 \times 2}{1} \frac{J}{CA}$$

$$F_{AO} = C_{AO} v_0$$

$\therefore CA = CB$,
 (equimolar)
 thus $C_A C_B = C^2$

$$D_a =$$

$$\frac{10}{e^{-10}}$$

$$X_{PFR} = \frac{10}{e^{-10}}$$

$$\frac{10}{e^{-10}} = 0.9999$$

$$\frac{10}{C_{AO}} \left(\frac{1}{e^{-10}} - 1 \right) = \int_0^x \frac{dx}{k C_{AO} (1-x)^2}$$

$$t = \left(\frac{1}{k C_{AO}} \right) \int_0^x \frac{dx}{(1-x)^2}$$

$$-\frac{1}{k C_{AO} t} = -\frac{1}{10} x^{-1} = (1-1)$$

Damkohler Number is used to calculate the Extent of Rxn.
 ↓
 property of system, depends upon entry condition

Homogeneous Liquid Phase Rxn :- $A + B \xrightarrow{\text{Products}}$

$$V = 2 \text{ lit}$$

$$r_A = 1 \text{ mol/l min}$$

$$C_{A_0} = C_{B_0} = 0.05 \text{ mol/l}$$

$$(a) X_{PFR}?$$

$$(b) X_{CSTR}?$$

$$(c) V_{CSTR} ? \text{ if } X_{CSTR} = X_{PFR}$$

A Hand

Soln:-

2nd Order Rxn

$$Da = \frac{(-r_{AO}) \cdot V}{F_{AO}}$$

$$\equiv \frac{100 \cdot C_{AO} C_{BO} \cdot V}{C_{AO} \cdot r_{AO}} = \frac{100 \times 0.05 \times 2}{1}$$

$$F_{AO} = C_{AO} r_{AO}$$

$\therefore C_A = C_B$,
 (equimolar)
 thus $C_A C_B = C^2$

\equiv

$$Da = \frac{10}{e^{-10}}$$

$$X_{PFR} = \frac{1}{1 + e^{-10}}$$

$$\frac{1}{1 + e^{-10}} = 0.9999$$

$$\frac{T}{Ca_0} \left(\frac{Ca_0 - t}{Ca_0 - 1} \right) = \int_0^x \frac{dx}{k Ca_0^2 (1-x)^2}$$

$$t = \frac{Ca_0 - 1}{k Ca_0} \int_0^x \frac{dx}{(1-x)^2}$$

$$Da = \frac{k Ca_0 T}{Ca_0 - 1} = \frac{-1}{1-x} \Big|_0^x = \left(\frac{1}{1-x} \right)$$

- Rxn.

$$10 = 1 - \frac{1}{1-x}$$

$$\frac{1}{1-x} = 9$$

$$-\frac{1}{9} = 1-x$$

$$x = 1 + \frac{1}{9}$$

$$Da = -\frac{1}{1-x} - \left[-\frac{1}{+} \right]$$

$$Da = 1 - \frac{1}{1-x}$$

$$\frac{1}{1-x} = (1-Da)$$

$$\frac{1}{1-Da} = 1-x$$

$$\boxed{x_1 = 1 - \frac{1}{1-Da}}$$

$$Da = \frac{1}{1-x} - 1$$

$$(Da+1) = \frac{1}{1-x}$$

$$\frac{1}{Da+1} = 1-x$$

$$x = 1 - \frac{1}{Da+1}$$

$$X_{PFR} = 0.91$$

$$\# X_{CSTR} = 0.91$$

AT-

$\# \#$ To find V_{CSTR} if $X_{CSTR} = \underline{X_{PFR}}$

$$\frac{\underline{I}}{CA_0} = \frac{V}{FA_0} = \frac{X_{A,e}}{(-\gamma_A)}$$

$$-\gamma_A = k CA_0^2$$

$$Da = k I CA_0$$

$$\frac{\underline{I}}{CA_0} = \frac{X_{A,e}}{k CA_0 \cdot CA_0}$$

$$Da = \underline{X_{A,e}} = 0.91 = \frac{V}{FA_0}$$

$$F_{CA_0} = CA_0 \times 20$$

$$V = 0.91 \times L \times 0.05$$

Batch Reactor

PFR

CSTR or MFR

or
Backmix Reactor

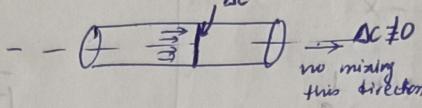
uniform (Ideal)

mixing in all directions.

1. mixing:
uniform (Ideal)

no mixing axially
(ideal)

$$\Delta C = 0$$



Complete mixing radially.

2. Basis of Design Input

=> clearing / loading

Other Parameters
Initial moles : N_{AO}
Unloading

Total moles : N_{TO}

P_{total} Reaction

Reaction kinetics

some thing

\rightarrow mass flow Rate (F_i)
Volumetric flow Rate (V_i)

$\rightarrow C_{AO}$
 \rightarrow mass flow rate
 $\rightarrow P_{total}, T_{req.}$

\rightarrow Extent of
Reaction (X_f)

\Rightarrow Reaction kinetics

$$t_{PFR} = \frac{C_{AO}}{r_A} \int_{N_i}^{N_f} \frac{dx}{x}$$

$$t_{CSTR} = \frac{V_{CSTR}}{V_{CSTR} - r_A t_{CSTR}}$$

$$t_{CSTR} = \frac{C_{AO} X}{r_A}$$

3. Design Output

Volume
or time

4. Not a Continuous

Reactor

Unsteady State

Continuous
Reactor

SS

Continuous
Reactor

SS

EX 4.1 (Jm)

In Non Ideal

The y . com
different

DO JM Smi

Significance of S & T

Space Velocity

space time.

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

$$T \rightarrow \text{unit (hr}^{-1}\text{)}$$

$$S \rightarrow \text{unit } \left(\frac{\text{m}^3\text{ hr}^{-1}}{\text{m}^3\text{ s}^{-1}} \right)$$

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

$$T = \frac{V_{\text{reactor}}}{V_{\text{total}}} = \frac{\text{m}^3 \text{ of Reactor Volume}}{\text{m}^3/\text{h} \text{ of Reactant Stream, coming into the reactor to be processed.}}$$

Defnition of Ideal Reactor:
When each reactant molecule spends equal amount of time Inside the Reactor.

$$S = \frac{\text{m}^3/\text{hr} \text{ of Reactant Stream that can be processed}}{\text{m}^3 \text{ of reactor volume}}$$

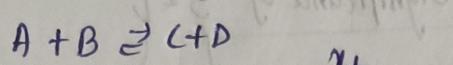
EX 4.1 (Jm Smith)

residence

In Non Ideal Reactor when there will be a distribution of residence time.
The % conversion of the Reactant molecules will be different and we get a distribution of conversions.

** Do Jm Smith Examples.

Q4.2 Hint



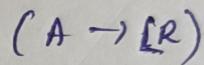
$$t_{\text{batch}} = \frac{N_A}{N_A - x_f} \int_0^{x_f} \frac{dx}{(1 - x_A) V}$$

$$k_f C_A C_B - k_b C_C C_D$$

Conversion & Concentration

table :-

$$C_A = N_A - N_A x_A$$



$$C_B = C_D - N_A x_A$$

$$C_C = C_D + N_A x_A$$

$$C_D = C_D + N_A x_A$$

$$t_{\text{batch}} = \frac{N_A}{N_A - x_f} \int_0^{x_f} \frac{dx}{V_D \left(k_f N_A (1 - x_A) (C_B - N_A x_A) - k_b N_A^2 x_A^2 \right)}$$

(continued on L) 2.11 x 3

$$-r_A =$$

$$C_A =$$

$$V =$$

$$w_D =$$

$$D_A =$$

For 2nd

Altitude

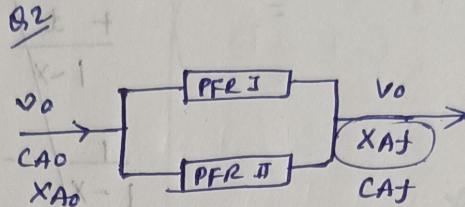
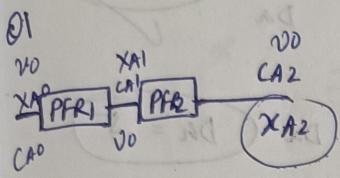
multiple Reactors

Series

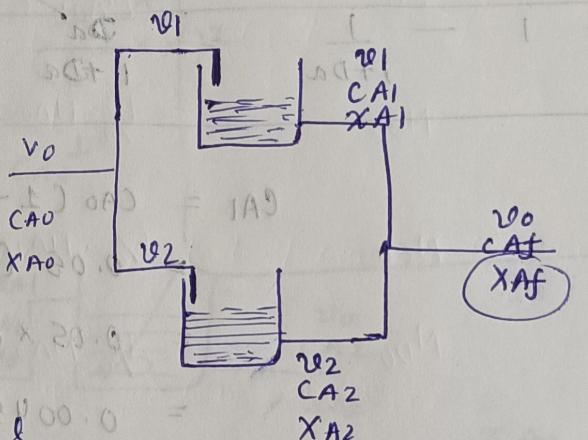
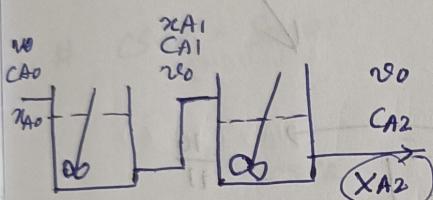
Parallel & Combination of MFR, PFR.

Parallel

Combination of MFR, PFR.



MFR.



$$-r_A = 100 \text{ mol CB.} \cdot \frac{l}{\text{min}}$$

$$C_{A0} = C_{B0} = 0.05 \frac{\text{mol}}{\text{lt}}$$

$$V = 2 \text{ lt}$$

$$\dot{V}_0 = 1 \text{ lt/min}$$

$$Da = k_D C_{A0}^{n-1}$$

For 2nd Order CSTR :-

$$Da_{CSTR} = \frac{X_A}{(1-X_A)^2}$$

Attempt
Soln Q1

X_{A1} (to find out)

$$Da_{PFR} = \frac{X_A}{(1-X_A)} \cdot$$

$$\begin{aligned} \rightarrow Da &= - \frac{(r_{A0})V}{F_{A0}} = \frac{100 (C_{A0}^2) V}{C_{A0} \times 200} \\ &= 100 K_0 \cdot 0.05 \times 2/1 = \frac{100 C_{A0} \cdot V}{V_0} \end{aligned}$$

Find out the circled quantities

$$L = \frac{V}{2D_a}$$

$$2D_a + 1 = \frac{1}{1-x}$$

$$1-x = \frac{1}{2D_a + 1}$$

$$1 - \frac{1}{2D_a + 1} = x$$

$$x = \frac{2D_a}{2D_a + 1}$$

$$\frac{x}{1-x} = D_a$$

situated
at outlet
of distillate

In PFR the overall conversion remains the same.

$$D_a = \frac{x_1}{1-x_1} = \frac{100 \times 1 \times 0.05}{1-0.05} = 5$$

$$x = 5(1-x)$$

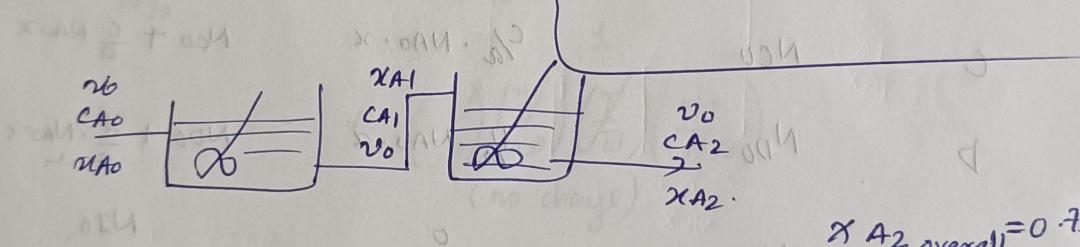
$$x = \frac{5}{6}$$

$$x = 0.833$$

CSTR - Series

$$D_a_{CSTR} = \frac{x_A}{(1-x_A)^2}$$

$$D_a = K T C A_0^{-1}$$



$$x_{A2\text{ overall}} = 0.73$$

$$D_a = \frac{100 \times 2}{2x+1} \times 0.05$$

$$\equiv 5$$

$$S = \frac{x_1^2}{(1-x_1)^2}$$

$$S(1+x^2 - 2x) = x$$

$$S + 5x^2 - 10x = x$$

$$5x^2 - 11x + 5 = 0$$

$$x = \frac{11 \pm \sqrt{121 - 100}}{10}$$

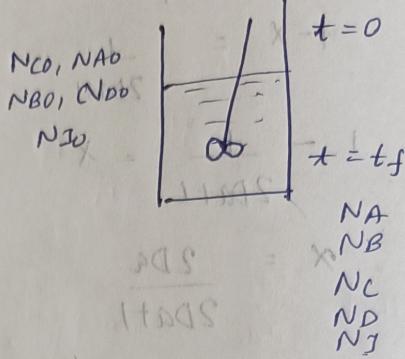
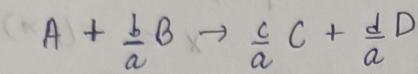
$$x_1 = \frac{11 \pm \sqrt{21}}{10} = 0.64$$

$4 \times 5 \approx 20$

Stoichiometric
Table for
Batch System

Batch System

Harold will tell
initial amounts



Species	Initial	Change Δn	Remaining
A	NAO	$-NAO \cdot x$	$NAO(1-x)$
B	NBO	$-\frac{b}{a} NAO \cdot x$	$NBO - \frac{b}{a} NAO \cdot x$
C	NCO	$\frac{c}{a} \cdot NAO \cdot x$	$NCO + \frac{c}{a} NAO \cdot x$
D	ND0	$\frac{d}{a} \cdot NAO \cdot x$	$ND0 + \frac{d}{a} \cdot NAO \cdot x$
NI0		0	NI0

$$N_0 = NAO + NBO + NCO + ND0 + NI0$$

$$N_t = NAO + NBO + NCO + ND0 + NI0$$

$$NBO \approx N_t \approx N_0 + NAO \cdot x \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \right)$$

$$- NAO \left(-1 + \frac{b}{a} + \frac{d}{a} \right)$$

$$\Delta n = \frac{\text{change in total no' of moles}}{\text{mole of A reacted}}$$

When can

but

Batch with

at $t =$

at t

NT

$$\frac{NT}{N_0}$$

also

E

When can volume change?

If we change P, T, n

but $T \Rightarrow$ unchanged (Isothermal)

$P \Rightarrow$ unchanged

$n \Rightarrow$ changes.

Batch with Variable Volume

$$\text{at } t=0 \quad P_0 V_0 = Z_0 N_{T_0} R T_0$$

$$\text{at } t=t_f \quad PV = Z N_T RT$$

$$N_T = N_{T_0} + N_{A_0} \times S \cdot x$$

$$\frac{N_T}{N_{T_0}} = 1 + \frac{N_{A_0} \times S \cdot x}{N_{T_0}}$$

$$\text{also } V = V_0 \left(\frac{P}{P_0} \right) \left(\frac{T}{T_0} \right) \left(\frac{N_T}{N_{T_0}} \right) \quad (\text{no change})$$

$$V = V_0 \cdot \left(1 + S \cdot \frac{N_{A_0} x}{N_{T_0}} \right)$$

$$V = V_0 \left(1 + \underbrace{S \gamma_A}_1 x \right)$$

$$V = V_0 \left(1 + \varepsilon_A x \right)$$

$$\therefore \varepsilon = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \right) \times \left(\frac{N_{A_0}}{N_T} \right) \hookrightarrow \gamma_{A_0} =$$

$$\epsilon = \frac{N_T - N_{T0}}{N_{T0} \cdot x}$$

valid for batch & flow reactors.

$$x = 1 \rightarrow \epsilon = \frac{N_T - N_{T0}}{N_{T0}}$$

Do similar procedure for flow system.

$$N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt}$$

$$N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt}$$

$$N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt}$$

$$N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt} \quad \text{or} \quad N_T = N_{T0} e^{kt}$$

$$\left(\frac{N_T}{N_{T0}} \right) \left(\frac{N_T}{N_{T0}} \right) \left(\frac{N_T}{N_{T0}} \right) \left(\frac{N_T}{N_{T0}} \right) \text{ or } \left(\frac{N_T}{N_{T0}} \right)^4 \text{ or } \left(\frac{N_T}{N_{T0}} \right)^4$$

$$\left(\frac{N_T}{N_{T0}} \right)^4 \text{ or } \left(\frac{N_T}{N_{T0}} \right)^4$$

$$\left(\frac{N_T}{N_{T0}} \right)^4 \text{ or } \left(\frac{N_T}{N_{T0}} \right)^4$$

$$\left(\frac{N_T}{N_{T0}} \right)^4 \times \left(\frac{N_T}{N_{T0}} \right)^4$$

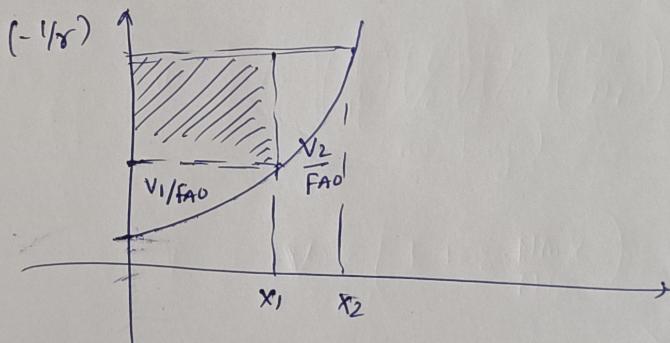
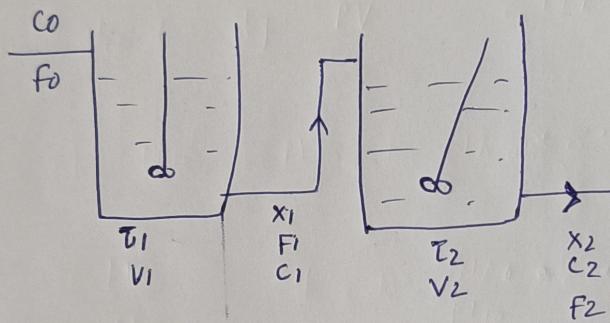
Liver Ch

$$\frac{C_0}{F_0}$$

①

②

Unversial
Ch-6



- ① How to arrange two unequal size Reactors to minimise volume for a given conv.
- ② to maximise the conv. for a given Volume,