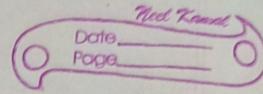
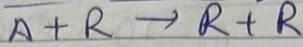


For an autocatalytic run
Compound A is a catalyst.

$\therefore -k_1 = k_{CA} C_R$



→ Optimum Recycle Ratio for an Autocatalytic Run



$$-k_A = k_{CA} C_R$$

$K = 0.1 \text{ lt/mol min}$, reactor.

$$C_A = 10 \text{ mol/l}$$

Recycle

(PFR).

$$C_{R_0} = 0$$

$$v_0 = 1 \text{ lt/min.}$$

$$X_{Ap} = 90\%$$

Ideal PFR $R \rightarrow 0$

$R \rightarrow \infty$
no effect
use of recycle
 $\therefore k_A = k_{CA}$.

Ideal CSTR

$R \rightarrow MFR$

- ① find the recycle rate which will minimize the size of reactor, find the volume.

② $v_{PFR} = ?$ when $R = 5$.

③ $R = \infty, v = ?$; $R = 0, v = ?$
(MFR) (ideal PFR).

Ans. $\frac{V}{F_{A_0}} = (R+1) \int_{-\frac{R}{R+1} X_{Ap}}^{X_{Ap}} \frac{dx_A}{(-k_A)}$

$$\frac{d(V/F_{A_0})}{dR} = 0 \quad \text{for } R \text{ min}$$

$$\frac{d}{dR} \left(\frac{V}{F_{A_0}} \right) = 0 \quad \Rightarrow f(R) = 0.$$

Solve by iteration
get $R = ?$ get $V = ?$

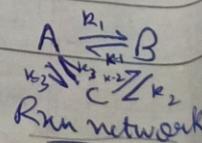
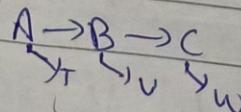
$$\begin{aligned} -k_A &= k_{CA} C_R \\ &= k C_{A_0}^2 (1-X_A). \end{aligned}$$

Multiple Reactions

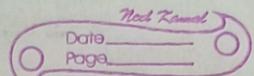
Series Run (consecutive Run).

Parallel Run (competitive Run)

3) Series-parallel run



branched Rmn
 eq. of Rmn network → enzymatic, conversion, some polymers
 short/parallel
 type of reactant → yield, selectivity
 well defined product
 request for more than product
 Reversible - Irreversible series Rmn
 Reversible - Irreversible Parallel Rmn



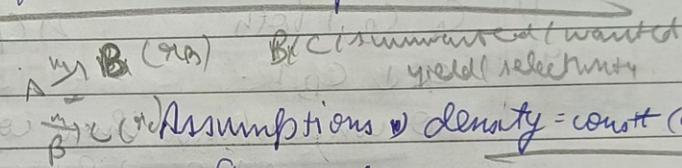
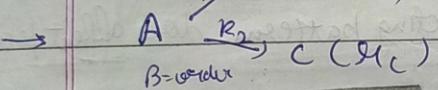
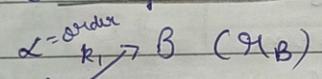
Rmn network - branch of series - parallel Rmn.
 eg. of such Rmn network include (i) Biochemical Rmn (enzymatic)
 2) Polymer synthesis Rmn; 3) Drug Industry, 4) Combustion

\rightarrow yield of a rmn ; selectivity of a rmn \rightarrow imp. free single rmn.
 (since only single product).

\rightarrow Based on kinetics & temp of a rmn

k_1 , may or may not be $= k_2$

thus we define yield of a rmn & selectivity of a rmn w.r.t desired products.



(i) Assumptions 1) density = const (c = q)
2) first order

$$-\eta_A = \eta_B + \eta_C$$

$$\left(-\frac{dc_A}{dt} \right) = \frac{dc_B}{dt} + \frac{dc_C}{dt}$$

3) liq phase rmn (const. density)

$$\eta_A = \eta_B + \eta_C$$

Assumption
1) density const
2) pure comp
3) liq. phase

$\alpha > \beta$ \rightarrow product distribution ; yield of desired prod \rightarrow based on type
of reactor in which rmn takes place

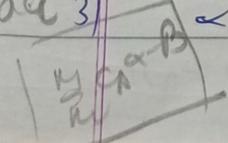
$$\eta_B = \frac{dc_B/dt}{dc/dt} = \frac{dc_B}{dc} = \frac{k_1 c_A^\alpha}{k_2 c^\beta} = \frac{R_1 c_A^{\alpha-\beta}}{R_2}$$

Based on values of α & β

$\alpha > \beta \rightarrow$ High η_B , if c_A is high.

$\alpha < \beta \rightarrow$ low η_B , if c_A is low

$\alpha = \beta \rightarrow$ no matter



for high C_A
 $\alpha > \beta$
 $\rightarrow PFR + Batch \rightarrow t_{batch} = T$
 1) High pressure
 2) Inert dilution
 3) Constant conversion
 $\rightarrow PFR$ if $x_B > x_C$ $PFR = \text{infinite CSTR}$
 for high x_B $R_1 + R_2 \rightarrow f(T)$
 for low x_B \rightarrow isomerizable single product by changing T
 for low x_B \rightarrow polymerization or CSTR
 for low x_B \rightarrow many extraneous species
 for low x_B \rightarrow less inert

on varying T
 $\frac{R_1}{R_2}$
 $\frac{x_B}{x_C}$
 $\frac{PFR}{CSTR}$
 $\frac{t_{batch}}{T}$
 $\frac{\text{Rate}}{\text{Rate}}$
 $\frac{\text{Page}}{\text{Page}}$

for high rate of B , R_1 and R_2 can be varied, but
 considering isothermal cond., R_1 & R_2 not varying (assumed)

$\alpha > \beta$ for high C_A 1) PFR. 2) Pressure is high 3) Less Inert

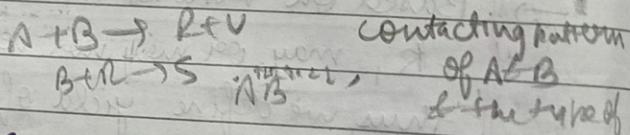
4) Maintaining low conversion

$x_B > x_C$
 high C_A $\rightarrow PFR$ $\therefore t_{batch} = T_{PFR}$ (for const. volume V).
 \rightarrow time with x_B , t_{batch} must be less.

$\alpha < \beta$ for low C_A 1) CSTR 2) Less Pressure 3) More Inert

$x_B > x_C$
 $C_A \rightarrow CSTR$ (sideways mixing)

\rightarrow low pressure
 mixing of reactants & type of reactor is imp. for multiple
 streams.



1) $C_A, C_B \uparrow$ both

\rightarrow Contacting Pattern.

$A + B \rightarrow R + V$

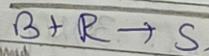
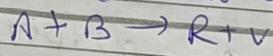
2) $C_A, C_B \downarrow$ both

$C_A \downarrow, C_B \uparrow$.

3) $C_A \uparrow, C_B \downarrow$

very
less

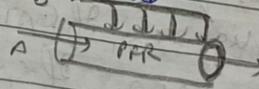
\rightarrow understand how contacting pattern does affect product yield



$C_A, C_B \uparrow$ both \rightarrow initially present (both C_A & C_B) \rightarrow both
 Reactants stream mixed in PFR / Batch.

Initially present
 (Batch / PFR). $\Rightarrow PFR$

$C_A, C_B \downarrow$ both \rightarrow both reactants stream mixed in MFR or CSTR
 $C_A \uparrow, C_B \downarrow \rightarrow$ imp PFR; B added sideways (B is intermittent;
 B added in pulses). Start with A & add slowly.



$C_A, C_B \rightarrow CSTR$

ΔP_{side}

$C_A, C_B \rightarrow CSTR$

ΔP_{side}

$B \rightarrow CSTR$

$$\phi_{PFR} = ? \quad \phi_{MFR} = ?$$

$$\phi_{PFR} = \frac{dc_R}{-dC_A}$$

$$\psi_{PFR} = \frac{dc_R}{-dC_A}$$

$$\int dc_R = \int \psi dC_A$$

$$\int dc_R = \int \psi dC_A$$

$$C_{Rf} = \int_{C_A}^{C_A} \psi dC_A$$

$$\phi = C_{Rf}$$

$$C_A - C_{Af}$$

$$\int_{C_A - C_{Af}}^{C_A} \psi dC_A$$

In PFR, the com
drop is gradual

$$\rightarrow \phi = \frac{1}{\int_{C_A - C_{Af}}^{C_A} \psi dC_A}$$

$$\phi_{PFR} \cdot \phi_{MFR}$$

$$\phi_{PFR} = \frac{dc_R}{-dC_A}$$

$$\int dc_R = \int \psi dC_A$$

$$C_{Rf} = \int_{C_A}^{C_A} \psi dC_A$$

$$\phi = \frac{C_A}{C_A - C_{Af}}$$

$$\phi = \frac{1}{\int_{C_A - C_{Af}}^{C_A} \psi dC_A}$$

ϕ_{PFR} com drop

in CSTR
many com drops
needed

in CSTR: $C_A = C_A$

$$\phi_{MFR}$$

$$\psi_{MFR} = \frac{dc_R}{-dC_A}$$

$$= \frac{C_{Rf}}{C_A}$$

$$= \frac{C_{Rf}}{\int_{C_A - C_{Af}}^{C_A} \psi dC_A}$$

1.2
→ Eq:

For PFR
 $\psi_{PFR} = \int_{C_A}^{C_A} \psi dC_A$

$\psi(C_A) = \frac{dc_R}{-dC_A}$

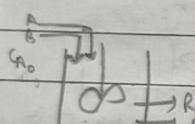
Ans. 1)

depends
on B way

more
PFR

Req. flow B
PFR \rightarrow more

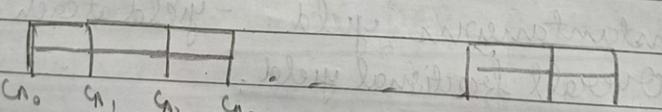
$\phi = \text{less}$
than MFR



For MFR ($\because C_A$ is CSTR is same)

$$\phi_{MFR} = \psi \text{ at } C_{Af} = \frac{dc_R}{-dC_A} \Big|_{C_{Af}}$$

For N reactors MFR in series.



$$\phi_{MFR} = \psi_{1, MFR} \psi_{2, MFR} \dots \psi_{N, MFR}$$

$$\phi_{MFR} = \psi_{1, MFR} \psi_{2, MFR} \dots \psi_{N, MFR}$$

$$\phi_{MFR} = \frac{C_{Rf}}{C_A - C_{Af}}$$

$$\psi_{1, MFR} = \frac{dc_R}{-dC_A} = \frac{C_{Rf}}{C_A - C_{Af}}$$

$$\phi_{MFR} = \frac{C_{Rf}}{C_A - C_{Af}} = \frac{C_{Rf}}{\int_{C_A - C_{Af}}^{C_A} \psi dC_A}$$

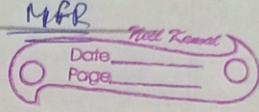
$$\psi_{1, MFR} = \psi \text{ at } C_A = \frac{C_{Rf}}{\int_{C_A - C_{Af}}^{C_A} \psi dC_A}$$

$$\phi_{PFR} = \frac{C_{Rf}}{\int_{C_A - C_{Af}}^{C_A} \psi dC_A}$$

$$= \frac{C_{Rf}}{\int_{C_A - C_{Af}}^{C_A} \psi dC_A}$$

$$\Psi = \frac{\partial \text{desired}}{\partial \text{reacted}}$$

$$\Phi = \int \Psi dC_A \quad \Phi = \Psi \text{ at } C_f$$



~~Partial~~ ~~Conc.~~

$$C_{sf} + C_{sf} = \Delta C_A = C_0 - C_f$$

~~Initial Conc.~~

$$C_{sf} = 0.9 + 0.32 = 1.28$$

$$C_{sf} = \underline{6.12}$$

$$C_{sf} + C_{sf} = \Delta C_A = C_0 - C_f$$

$$100.9 = 9$$

$$\text{MFR} \quad \text{MFR} = \Psi \text{ at } C_f = \frac{dC_f}{dC_A} \quad \frac{C_0 - C_f}{C_f^{0.5}} = 0.5$$

$$C_f = 9 \times 0.5 = 4.5$$

$$C_{sf} = 9 \times 0.5 = 4.5$$

c). PFR - MFR mixed,

$C_A \rightarrow$ gradually $\rightarrow A$ as PFR
 B as MFR $\sim C_B$ low \rightarrow conⁿ reaches final conⁿ. assume
as soon as A & B enters it becomes 10 & 10 \rightarrow and soon B converts to B at final point i.e. 1, thus $C_{Bf} \downarrow$ drastically

\Rightarrow adding
side wise
and slowly
 \downarrow
conⁿ level
to be kept
as low as
possible

to T Φ . $C_{sf} \rightarrow 19 (10+9)$.

$$\Psi = \frac{C_A^{0.5}}{C_A}$$

$$= \frac{C_A^{0.5} \cdot C_B}{C_A \cdot C_B}$$

$$= 0.932$$

$$C_{Bf} \geq 0.932$$

$$C_A \cdot C_B$$

$$C_A = 19 \quad C_B = 1$$

$$C_B = 1 \quad C_A = 19$$

$$= 20$$

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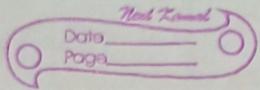
$$= 20$$

$$C_B = 19 \quad C_A = 1$$

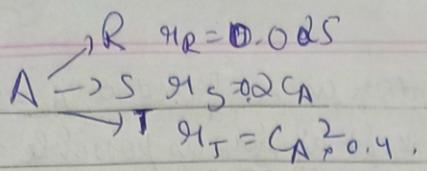
$$= 20$$

$$C_B = 19 \quad C_A = 1$$

$$= 20$$



Ques 7.3



Find minimal expected C_S for
isothermal operations.

a) in MFR

b) in PFR

c) Recycle to the feed at
 $(MFR + PFR)^{1/2}$.
 $C_{A0} = 2$
 \rightarrow PFR with an MFR.

$$\text{Ans} a) \Phi\left(\frac{S}{A}\right) = \Phi \text{ at } C_F$$

$$\cancel{\Psi\left(\frac{S}{A}\right) \propto S}$$

$$\Psi\left(\frac{S}{A}\right) = \frac{dCS/dt}{-dCA/dt}$$

$$\frac{2C_A}{1+2C_A+C_A^2} = \frac{0.2C_A}{(C_A+1)^2}$$

$$\text{MFR} = \frac{C_M}{C_0 - C_M} =$$

$$\Psi_{\text{MFR}} = \Psi_{C_F}$$

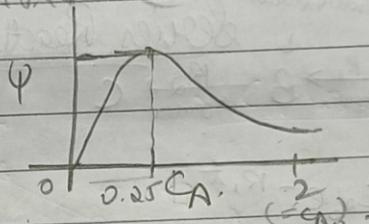
$$= \frac{8C_A}{(1+4C_A)^2}$$

$$\Psi\left(\frac{S}{A}\right) = \frac{dCS/dt}{-dCA/dt} = \frac{0.2C_A}{0.02C_A + C_A + 0.25} = \frac{8C_A}{(1+4C_A)^2}$$

for a given
 $MFR = 1$ area
under curve
area under
curve under PFR
is

Ψ_{MFR}

$$\Phi = \Psi_{\text{MFR}} = \frac{8C_A}{(1+4C_A)^2}$$



init

$$a) C_S = \Delta C_A * \Phi \text{ at } C_F.$$

$\Phi = 1$ (why) For MFR, area under curve has to be minimised

$\therefore \Phi \times \Delta C_A$ has to be minimised to maximise C_S .

corner
 $C_S \rightarrow$ area under
curve
has to be
minimised

$$C_S = (C_{A0} - C_{A_F}) \left[\frac{8C_A}{(1+4C_A)^2} \right].$$

$$\frac{dC_S}{dC_{A_F}} = 0$$

$$C_{A_F} = 0.2$$

For PFR all area under

$$\frac{dC_S}{dC_{A_F}} = 0$$

$$C_S = (2 - C_{A_F}) \left[\frac{8C_A}{(1+4C_A)^2} \right].$$

$$\frac{dC_S}{dC_{A_F}} = \frac{(1+4C_{A_F})^2 [16] - 16C_{A_F} [2(1+4C_{A_F})^4]}{(1+4C_{A_F})^4} - \frac{d8C_A^2}{(1+4C_{A_F})^2} = 0$$

MFR \rightarrow more
area than
PFR

\therefore more
conversion.

$$= C_{A_F} = 0.2 \approx (1/5)$$

$$C_S = 8/9$$

$$C_{A_F} = 0$$

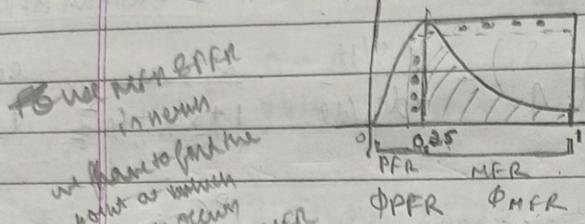
61. For PFR we assume all area under curve \therefore all conversion of

$$A \quad \therefore C_{A_F} = 0$$

$$\therefore C_{S_F} = 0.654$$

- c). $\therefore C_p^2$ in denominator as compared to C_A .
 ∴ C_p must be kept as low as possible → MFR has max area under curve.
 ∴ Find the point at which minimum C_p occurs till that
 operate under MFR i.e. till $C_p = \underline{0.25}$ (here).

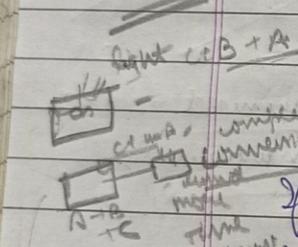
(Case I)



$$C_{Sp} = 0.972.$$

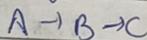


In that case overall distribution would be non for MFR.

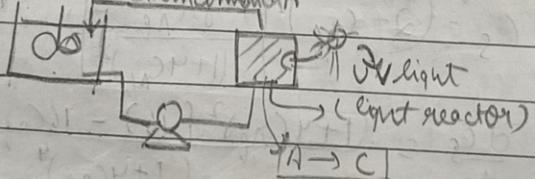


If B is undesired, we have to see the way through which min. B, while max. C is formed.

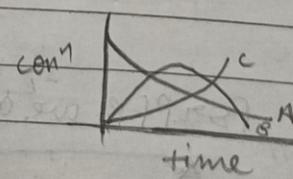
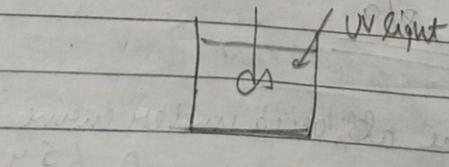
→ Case 1 light reactor - UV reactors etc, (sun starts when)



(+ unconverted A)



Case 2 → whole reactor exposed to light.



parallel sun → the underlying nature of the system → min. total area → for series → PFR → strong min. is not there → C is PFR C parallel underlying

find the T_{max} for min. intermediate conc. given graph

~~AIR → S~~

~~P → R → S~~
Slow completion of P into S

- ∴ to control the intermediate period -
 the type of reactor without mixing is very imp.
 ∴ the two streams with stiff comp. Should not happen
Note: to control intermediate period
Data to control
Poga

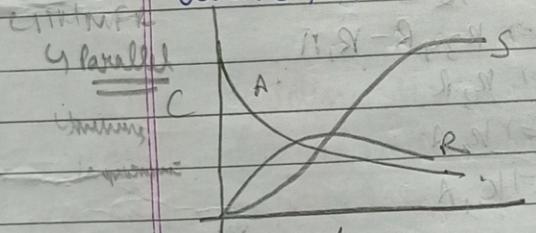
Case I

In order to control the ^{intermediate} prod. distribution in a series reactor
 mixing of two streams with different composition should not happens

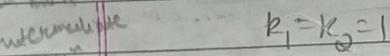
→ for parallel reactor - conⁿ of A is important
 For series → intermediate prod. conⁿ is imp.
 For PFR or batch - better to control intermediate prod.
 since mixing is not prominent (batch :: we can control batch time)
 CSTR - better for control conⁿ of reactant, product :: mixing is prominent.
 For series - intermediate prod. conⁿ is imp.

∴ PFR → series
 find t_{opt} for C_B max/min. Batch time PFR time MFR time
 mixing is not prominent

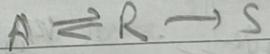
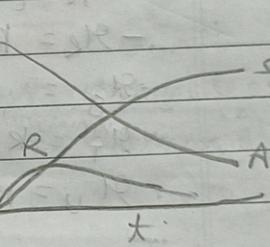
→ Write sum network



Find the t_{opt} for max/min. t
 w.r.t. intermediate conⁿ
 given graph below (sum network)

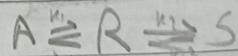
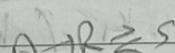
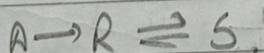
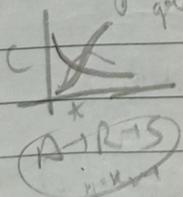


$$k_1 = k_2 = 1$$

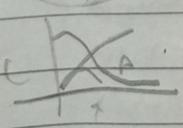


Slow depletion of A, non-interacting A & R

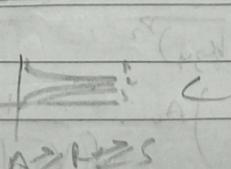
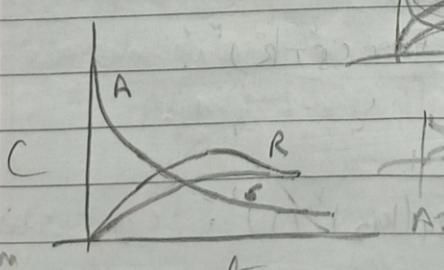
$$k_1 = k_2 = 1$$



$$\begin{aligned} g_{1F} &= k_1 C_A - k_1 C_R \\ &\approx k_2 C_R + k_2 C_S \\ g_{1E} &= k_1 C_A + k_2 C_S \\ &\approx k_2 C_R + k_2 C_S \end{aligned}$$

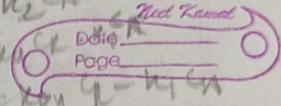
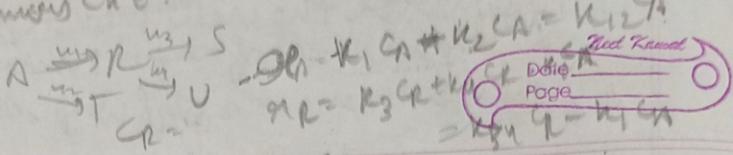


Slow depletion of A, non-interacting A & R



$$g_{1S} = \frac{C_A + C_S - 2C_R}{C_A - C_S}$$

Denbigh \rightarrow formers ch.

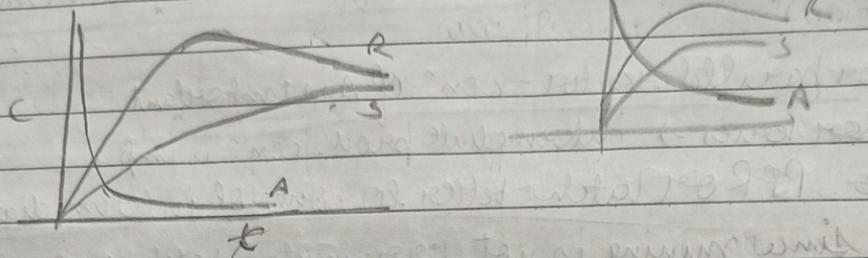


If $A \overset{k_1}{\rightarrow} R \overset{k_3}{\rightarrow} S$

$$R = k_3 A$$

$$dR = k_3 C_A \quad A \xrightarrow{k_1} R \xrightarrow{k_3} S$$

$$dR = k_3 C_A$$



$A \xrightarrow{k_1} R \xrightarrow{k_3} S \rightarrow$ In PFR; Recycle reactor is used

In the case of ~~homogeneous~~ the reactant formed a reaction; R promotes & more than.

Denbigh $\xrightarrow{k_1} A \xrightarrow{k_2} R \xrightarrow{k_3} S$ find $C_{R,\text{max}}$ & t_{max} in terms of state constant.

$$-\dot{R}_A = [R_1, A + R_2, A]$$

$$\Rightarrow R_{12} A \text{ and } R_1 A$$

$$-\dot{R}_R = R_3 R + R_4 R - R_1 A \Rightarrow R_3 R - R_1 A$$

$$-\dot{R}_S = R_3 R$$

$$= k_3 R$$

$$-\dot{R}_T = R_1 A$$

$$= k_1 A$$

$$-\dot{R}_U = R_4 R$$

$$= k_4 A$$

$$C_{R,\text{max}} = \int_{C_A}^{C_{R,\text{max}}} \Phi dC_A$$

n.w. check

$$\therefore R_{12} = k_1 + k_2$$

$$k_{34} = k_3 + k_4$$

$$t_{\text{max}} = \ln \left(\frac{k_{34}}{k_{12}} \right) \cdot (T \text{ for PFR})$$

$$R_{12} = \frac{k_{12} A}{k_{34} R - k_{12} A} dC_A$$

for batch & PFR.

$$C_{R,\text{max}} = C_{A_0} \cdot \frac{k_1}{k_{12}} \left(\frac{k_{12}}{k_{34}} \right)^{\frac{k_{34}}{k_{34}-k_{12}}}$$

$$\frac{dC_R}{dC_A} = 0 \text{ w.r.t. } C_A$$

for

$$t_{\text{max}} = \frac{1}{(k_{12}/k_{34})^{1/2}}$$

(for CSTR). $t_{\text{max}} = \ln \left(\frac{C_{A_0}}{C_{A_{\infty}}} \right) / \frac{k_{34}}{k_{12}}$

CSTR,

$$C_{R,\text{max}} = \left(\frac{R_1}{R_{12}} \right) A_0 \cdot \frac{1}{((k_{34}/k_{12})^{1/2} + 1)^2}$$

$$C_A = (C_{A_0} - C_{A_{\infty}}) \Phi + C_{A_{\infty}}$$

$t_{\text{batch}} = \frac{1}{k_{34}}$

$t_{\text{PFR}} = \frac{V}{k_{34} A}$

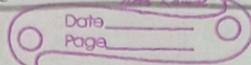
Residence time - the time molecules spend in a reactor. Not all molecules are required to spend same time in the reactor.

Residence time = the amount of time a molecule spends in a reactor

Real Reactor

→ Residence time is varying or non uniform.

Non-Ideal Reactors



Imperfections in reactor → ↓ rate of conv

ideal reactor

→ Imperfections in reactor reduces rate of conv

ideal reactor → highest conversion always.

Imperfections → Residence time distribution.

Ideal Reactor
→ residence time of all molecules is same

Ideal Reactor - Reactor in which packets of elements spend same time in a reactor.

for a tracer molecule → molecule used to trace the time spent in a reactor.
tracer pulse input
the pulse given can be pulse or step.

If there is L.T. diff.

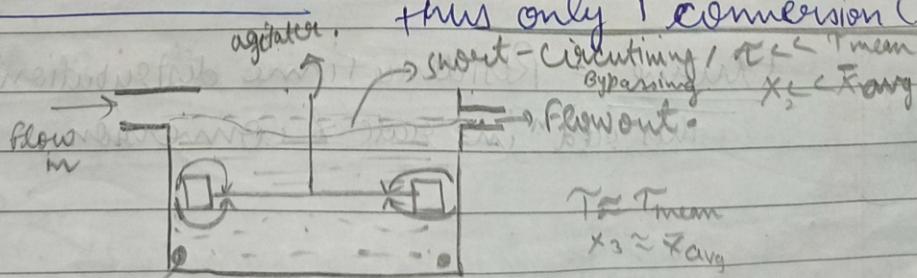
→ conversion is diff. parts of reactor will have diff. conversion.

Real reactor - T_{mean} = mean residence time / avg. residence time
= different batch have diff. T_{mean} .

(1) Real reactor T_{mean} - mean avg. Residence time thus we get a \bar{x}_{avg} .

Ideal reactor - $T = \text{constant}$ residence time → $x_1 = x_2 = \dots = x_n$.

thus only 1 conversion (x).



Stagnant region (remains even if $T \rightarrow \infty$)
 \therefore (in this region $x_i \rightarrow 1$)

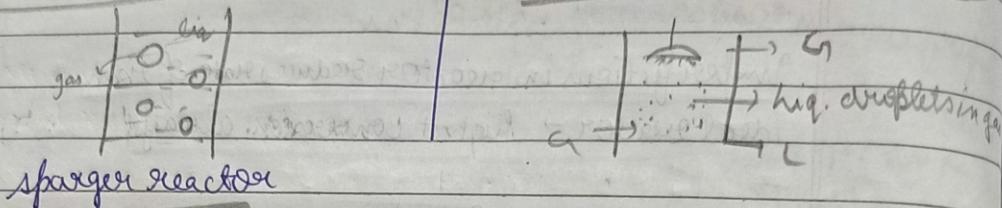
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gas can be bubbled in liquid phase
or liquid can be sprayed as drops.

2 ways of contact
gas-liquid contact liquid-liquid contact

→ gas-liquid imm. - 2 ways of contact.

gas is bubbled through liquid. / liquid sprayed through gas flow.



sparger reactor

- spray tower reactor

effect of different

→ channeling - very prevalent in 2 phase reactor also in packed bed imm. operation.

3-phase (solid-gas-liquid) reaction.

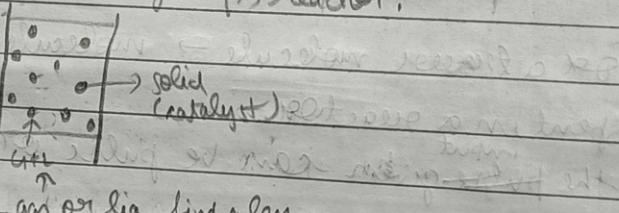
escaping of

gas

without

medium

contact



→ e.g. of channeling i.e. overall

resistance

difficult

channeling

channeling is more in 3 phase imm. lesser in single phase imm.

These anomalies reduces the rate of imm.

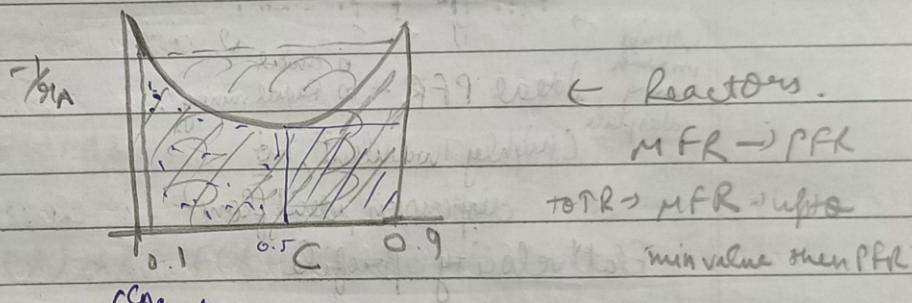
$$\bar{x} = \int_0^\infty x(t) E(t) dt.$$

$$\bar{x} = \int_0^\infty x(t) E(t) dt$$

Ecurve = Residence time distribution curve → reason for this "redn" in rate & conversion.

Q1) $C_{A_0} = 0.99 \quad C_{R_0} = 0.01 \quad R = 1 \text{ ft/min}$
 $C_{A_f} = 0.1 \quad C_{R_f} = 0.9$
 $C_A + C_R + C_{A_0} + C_{R_0} = C_A + C_{A_f} = 1$

| C_A | C_R | $\eta_A = k_C A / R$ | η_A |
|-------|-------|----------------------|----------|
| 0.99 | 0.01 | | |
| 0.8 | | | |
| 0.4 | | | |
| 0.3 | | | |
| 0.2 | | | |
| 0.1 | 0.9 | | |



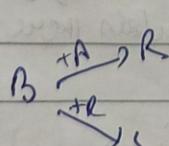
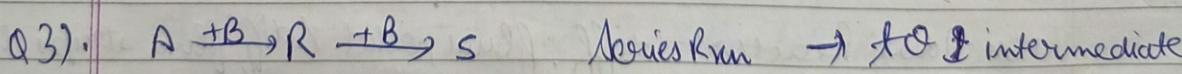
$$\tau_{PFR} = \frac{\int_{C_{A_0}}^{C_{A_f}} \frac{dC_A}{\eta_A}}{C_{A_0}}$$

Q2) MFR. $\varphi \left(\frac{C_R}{C_S} \right)$ - desired R $C_n \approx 0$

for $R < n$ for S .

conc of A .

$\therefore \underline{\text{CSTR/MFR.}}$



Desired $\frac{dt}{dt} = S$

Parallel Run.

mixing must not be done \therefore PFR

$B \rightarrow$ slowly (limiting reactant), low conc

$B \rightarrow$ quickly (excess), conc high

$\therefore A \uparrow \text{MFR}$ continuous. $B \uparrow \text{PFR}$ continuous.

nonconvolution

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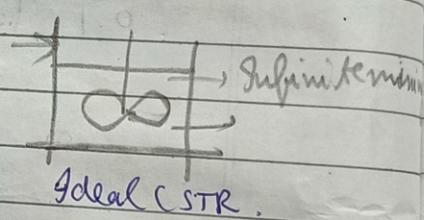
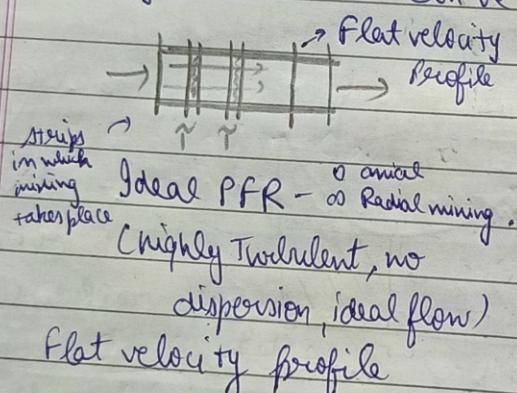
Ch 11, 11.1, 11.2 RTD / non-Ideal Reactors.

- Micromixing → micro reactor,
non-segregated fluids, micro fluids
- Macromixing → macro reactor
(segregated fluid) → macro fluids

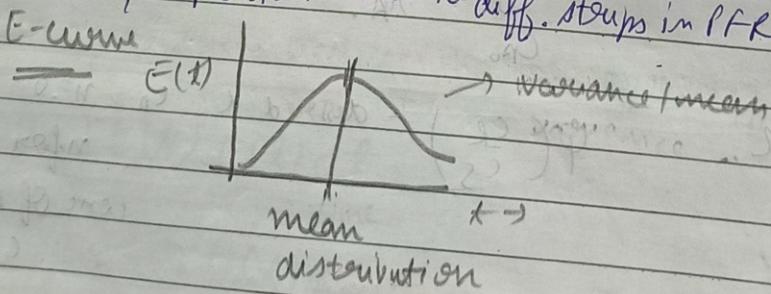
Mixing - gives idea of non-ideality

Extreme reactors. Ideal PFR

for any reactor RTD can be done.



Turbulence, dispersion leads to diff. strips in PFR having diff. τ_i



non-Ideal Reactor - diff. fluid pocket, 1/diff fluid strips have uneven mixing. \rightarrow within these packets there is infinite mixing

→ Criterion/Assumption for macromixing

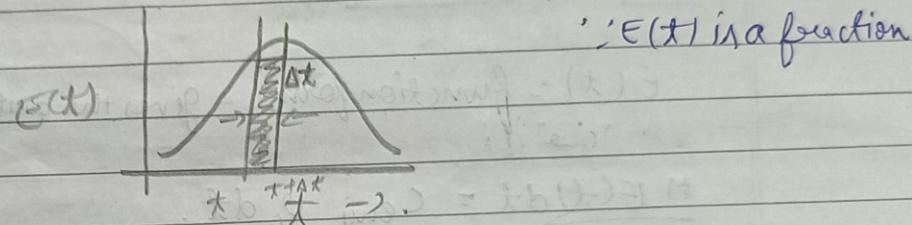
- 1) contents of the packets are infinitely mixed but two pockets don't mix with each other.

- 2) Each pockets has different τ but contents in a pocket have same τ .
- 3) Each pocket represents the same sum.

Only the diff. is the time which leads to diff. conversion.

PFR \rightarrow a macro reactor

MFR/CSTR \rightarrow a micro reactor \rightarrow \therefore mixing takes place.



$$\int_0^\infty E(t) dt = 1 \rightarrow E_{curve}$$

$$\int_0^t E(t) dt = F(t) \rightarrow F_{curve}$$

unit of $E(t) = \frac{\text{time}}{\text{time}}$

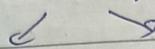
st. $E(t) =$ Fraction of fluid elements which spend time t and $t + \Delta t$.

$$\therefore \int_0^\infty E(t) dt, = \sum_{\Delta t} = 1$$

$F(t) =$ fraction of fluid elements which comes out of the reactor till ' t ' or have residence time $\leq t$

$1 - F(t) =$ fraction of fluid elements which is still in reactor till ' t '.

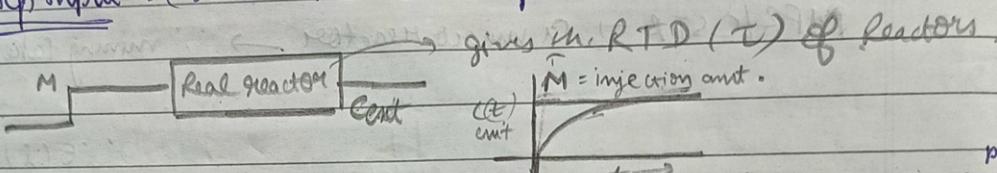
Determining RTD or E curve.
Tracer or injector molecule.
technique.



Step input Pulse.

If we try calculate RTD using tracer molecule we can't do it at same time.

→ Step Input. (selectant mol. can't be put)



$E(t)$ - function form - gives the dist. of t . → (an imp. design parameter).

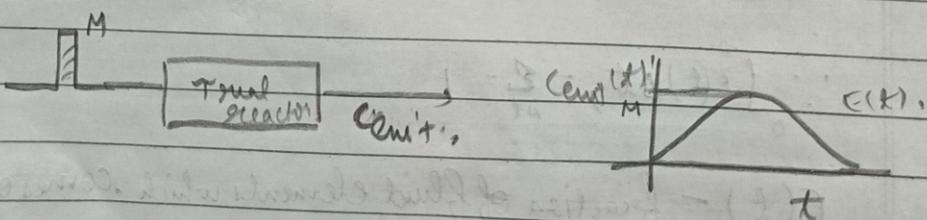
$$\frac{M \cdot E(t) \cdot dt}{\text{amt.}} = C_{\text{init}} \cdot v_0 \cdot dt.$$

amount (moles),

$F(t)$ = cumulative, $E(t)$ = distribution.

$$\frac{dF(t)}{dt} = E(t).$$

→ Pulse Input (Assuming pulse time is insignificant as compared to reactor time.)



Each curve is a characteristic curve for a reactor.

$E(t)$ = Pulse tech
 $F(t)$ = Step tech.

$$\frac{dF(t)}{dt} = E(t).$$

$$E(t) = \frac{C_{emit}(t)}{\int_0^t C_{emit}(t') dt'}$$

Data
C_{emit}

$$E(t) = \frac{C_{emit}(t)}{M/V_0}$$

$$\frac{M}{V_0} = \frac{\int_0^\infty C_{emit}(t) dt}{m^3/sec}$$

$$i.e. E(t) = \frac{C_{emit}(t)}{\int_0^\infty C_{emit}(t) dt}$$

| Expt. II: | | time (t), min | tracer output con ⁿ (pulse / gm / lt). |
|-----------|----|---------------|---|
| Leverage | 0 | | 0 |
| | 5 | | 3 |
| | 10 | | 5 |
| | 15 | | 5 |
| | 20 | | 4 |
| | 25 | | 2 |
| | 30 | | 1 |
| | 35 | | 0 |

$$\bar{t} = \text{mean residence time} = \frac{\sum t_i C_i \Delta t}{\sum C_i \Delta t} \quad \Delta t = \text{constant.}$$

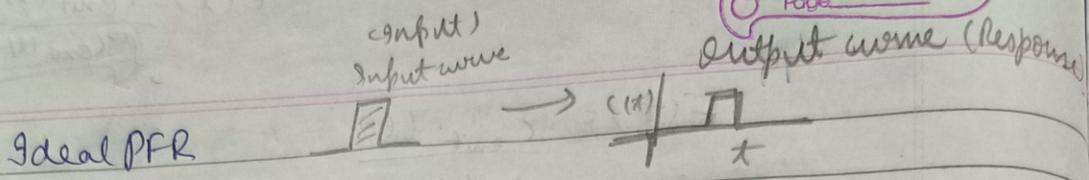
$$= \frac{\sum C_i t_i}{\sum C_i}$$

$$\bar{t}$$

$$= 15 \text{ min.}$$

Area under $C-t$ curve

$$\text{Actual area} = \sum C_i \Delta t \approx 100 \text{ gm. min lt.}$$



$$\int E(t) dt$$

Intrinsic quantity.

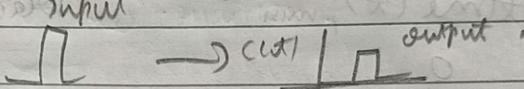
Intrinsic quantity can be \dot{H} , mass convection, momentum.

Ideal PFR

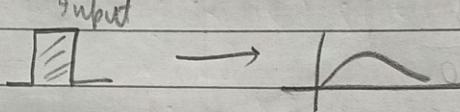
$$\int (X(t)) E(t) dt = \bar{X} = \text{avg conversion.}$$

$$\int \dot{H} E(t) dt = \bar{H} = .$$

For Ideal PFR



non-Ideal PFR



$$E(t) = S(t-\tau) \int_0^\infty \delta(t+\tau) dt \rightarrow \text{Ideal PFR.}$$

Impulse in $\int S(t-\tau) dt$ \rightarrow a dirac delta function.

For Ideal PFR, 1st order, elementary rxn.

$$\bar{X} = \int_0^\infty X(t) E(t) dt.$$

$$= \int_0^\infty X(t) S(t-\tau) dt.$$

$$= X(\tau)$$

$$= 1 - e^{-k\tau}$$

$$(X(t) = 1 - e^{-kt}).$$

Intrinsic kinetic
 $= n, R$

Given a real reactor

\bar{X} would be less than \bar{X} for ideal

Generally

$$\left(\frac{C_A}{C_{A0}} \right)_{\text{atexit}} = \int_0^\infty \left(\frac{C_A(t)}{C_{A0}} \right) * E(t) dt.$$

$$\frac{C_A}{C_{A0}} = \sum \frac{C_A}{C_{A0}} * E \Delta t.$$

$$E = \int_0^\infty t^n E(t) dt \Rightarrow n^{\text{th}} \text{ moment} . \quad \tau = \int_0^\infty t^2 E(t) dt$$

Note: *Var* variance
Date _____
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- Find out $E(t)$ for an ideal CSTR by impulse tech.
continuity eqn

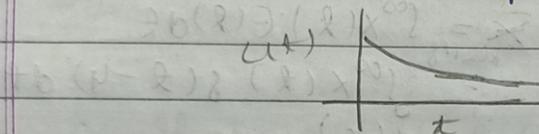
$$V \frac{dc_{\text{out}}}{dt} = \overset{\text{in}}{0} - \overset{\text{out}}{v_o c_{\text{out}}} + \text{reaction} \rightarrow \overset{\text{in}}{\int v_o} \overset{\text{out}}{c_{\text{out}}}$$

$\frac{dc_{\text{out}}}{dt}$
accumulated

$$\text{at } t=0 \quad c=c_0$$

$$c = c_0 e^{-t/\tau} = c_0 e^{-t\theta/v}$$

if input to an ideal CSTR is impulse
then output is an exponential decay curve.



$$E(t) = \frac{c_{\text{out}}}{\int_0^\infty c_{\text{out}}(t) dt}$$

$$= \frac{c_0 e^{-t/\tau}}{c_0 \left(\frac{-1}{\tau} \right) c_0 e^{-t/\tau} \Big|_0^\infty}$$

$$= \frac{1}{\tau} e^{-t/\tau} \quad 1/\tau e^{-t/\tau}$$

at $t \rightarrow \infty$ (because as it starts coming out slowly).
fill all out.

$c_{\text{out}}(t) = 0 \rightarrow$ all reactants have left the reactor.

$$E(t) = 0, \rightarrow$$

(ii) do the same for step input

$$\frac{dc_{\text{out}}}{dt} = Q c_{\text{in}} - Q c_{\text{out}}. \quad (\text{Ideal CSTR})$$

$$c(t) = ?$$

here we get $F(t)$
curve

$$\text{at } t=0, c_{\text{out}} = c_{\text{in}},$$

$$PFR: T/C_{A0} = \frac{V}{F_{A0}} = \int_0^{\infty} \frac{dx}{(-k_A)} =$$

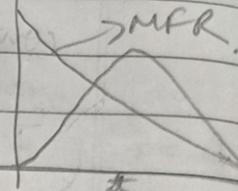
$$\text{Batch: } t = N_A \cdot \int_0^{x_{\text{max}}} \frac{dx}{(-k_A)}$$

$$MFR: \frac{T}{C_{A0}} = \frac{V}{F_{A0}} = \frac{x_{\text{AP}}}{(-k_A)} \cdot \frac{1}{1 - e^{-kt}} \cdot \frac{1}{t} e^{-t/\tau}$$

$$\bar{X}_{\text{ideal (STR)}} = \int_0^{\infty} x(t) E(t) dt$$

$$= \int_0^{\infty} (1 - e^{-kt}) \cdot \frac{1}{t} e^{-t/\tau} dt$$

$$= \frac{k\tau}{1 + k\tau} \quad \text{Ansatz.}$$



Assignment - 5

$$1) E(t) = 8(t-4), n=1^{\text{st}} \text{ order}, k=0.25.$$

Steady state & isothermal condition.

For ideal PFR

$$\bar{X}_{\text{ideal PFR}} = \int_0^{\infty} x(t) E(t) dt$$

$$= \int_0^{\infty} x(t) \delta(t-4) dt$$

$$= x(4)$$

$$\bar{X} = 1 - e^{-k\tau}$$

$$\bar{X} = 1 - e^{-0.25 \times 4}$$

$$\bar{X} = 1 - e^{-1} \Rightarrow (e-1)/e.$$

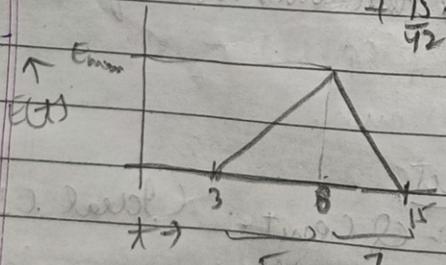
$$\bar{X}_{\text{ideal CSTR}} = \int_0^{\infty} x(t) \bar{E}(t) dt = \int_0^{\infty} (1 - e^{-kt}) \delta(t-4) dt.$$

$$= 1 - e^{-4k}$$

$$\frac{t^2 - t}{60} - \frac{t}{10} \Big|_0^8 = 1 - e^{-1}$$

$$+ \frac{15t}{92} - \frac{t^2}{84} \Big|_0^8$$

$$E(t) - 0 = \frac{E_{\text{max}} - 0}{8-3} (t-3).$$



$$E(t) - E_{\text{max}} = 0 - E_{\text{max}} (t-8)$$

$$E(t) = E_{\text{max}} \frac{(t-3)}{5} = \frac{E_{\text{max}} (8-t)}{7} + E_{\text{max}}$$

$$dE(t)/dt = 0$$

$$t_{\text{min}} = \int_0^{\infty} E(t) dt$$

$$8 \cdot 5 t_{\text{min}} = t_{\text{min}} = \int_0^8 \frac{1}{30} (t-3) dt + \int_8^{15} \frac{1}{42} (15-t) dt$$

$$E_{\text{max}} = V_6$$

3) Diffusion & min in porous catalyst
Rate eqⁿ and pore diff. in a single pore diff. & min in spherical catalyst pellet
Effectiveness factor
Estimation of diff. & min. limited regime.

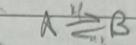
4) Non catalytic fluid-particle min
Intercept selection for model, unreacted core model for spherical particles of unchanged size, shrinking core model

Catalysis and catalytic min: Def., steps in a catalytic min, synthesising a rate law, mechanism, internal diffusion effect on heterogeneous min, rate limiting step, fundamental, external resistance to NT, mass transfer

Prof. Sonali Rxn. Eng.

Rate of min → consumption of reactant / Production of product with time

Equilibrium → no change in consumption of reactant or production of product with time.



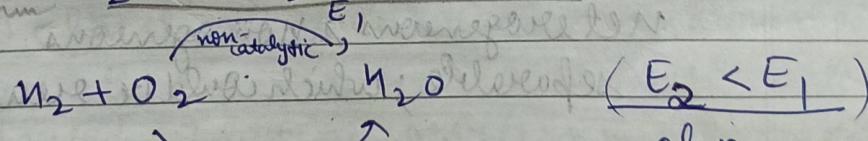
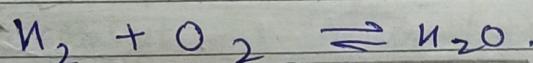
at eqⁿ $k_f = k_b$

$k_f C_A = k_b C_B$

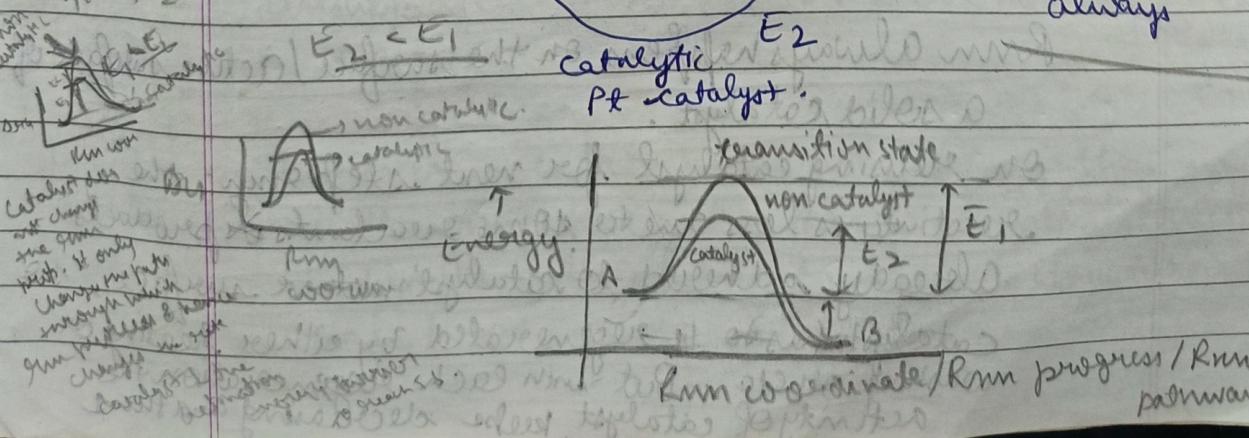
no change in concn. at a particular time

If the concn. at which this happens for B or A is high then we say the min is irreversible.

Catalyst changes the pathway through which min proceeds; catalyst chooses a path through which E_a is less as compared to non-catalytic min thus ↓ the time taken for min to reach eqⁿ.



always



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* 0.04 KB/S VOD 4G R 10

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