

Most catalyzed runs that are heterogeneous use this type of reactor \rightarrow to increase more yield.
 therefore conversion -

one/ First Pass conversion \rightarrow conversion along reactor
overall conversion - adding recycle then obtaining conversion.

The main parameter i.e. required to be found is R i.e., Recycle Ratio.

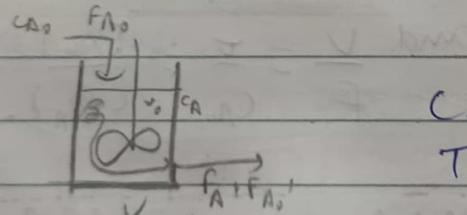
$$R = \text{Recycle ratio} = \frac{\text{volumetric flow rate of recycle stream}}{\text{volumetric flow rate of outlet}}$$

$$= \frac{\text{volume reacted}}{\text{volume sent out}} = \frac{V_3}{V_8} = \frac{R_{op}}{V_F}$$

Objective- rewrite design eq " ; range of R .

$R \rightarrow 0$ \rightarrow for PFR

$R \rightarrow \infty$ \rightarrow for CSTR (due to back mixing also called as back mix reactor).



CSTR gives lower rate than PFR

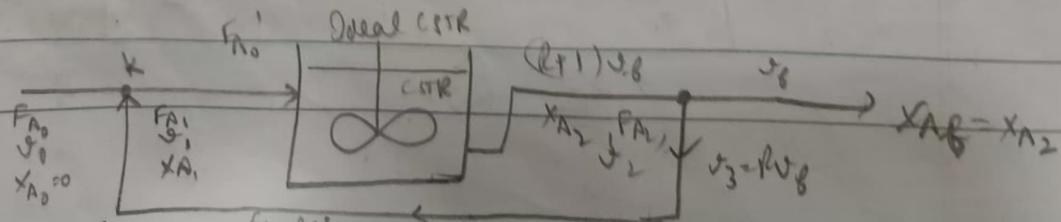
The connected reactor mixes with

a fresh reactor and instead of it coming out, due to stirring

it keeps getting mixed i.e. back mixing

\therefore CSTR is called as back mix reactor

$$R = [0; 0.5, \dots, 1000]$$



In perfectly mixed CSTR if recycle stream is added the final conversion does not change due to adding a perfectly mixed stream back into a perfectly mixed reaction mixture.
(e.g. just like taking out a bucket of water from sea).

→ Design eqn

$$\frac{V}{F_{A_0}'} = \int_{X_A}^{X_{A_p} = X_{A_2}} \frac{dX_A}{(1 - \epsilon_A)} \quad A \rightarrow \text{Products}$$

$$F_{A_p}' = F_{A_3} + F_{A_0}$$

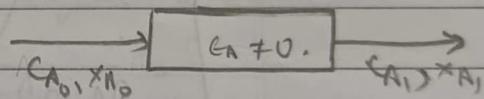
$F_{A_0}' = A$ which would have entered in an unconverted recycle stream

$$= R F_{A_0} + F_{A_0} = (R+1) F_{A_0}$$

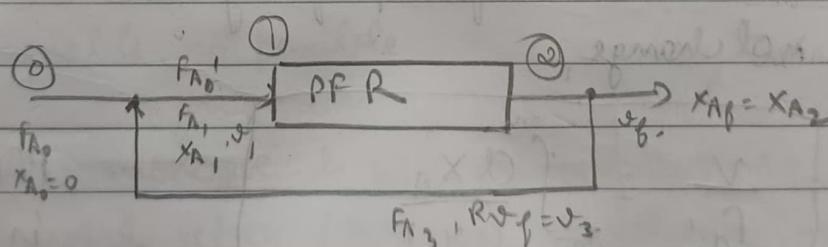
$$C_{A_1} = \frac{C_{A_0} (1 - X_{A_1})}{1 + R C_{A_1}}$$

X_{A_1} = unknown = [for gas phase & then $\epsilon_A \neq 0$]

$$X_{A_1} = 1 - \frac{C_{A_1}}{C_{A_0}} = \frac{C_{A_0}}{1 + R C_{A_1}}$$



In gen. in $\frac{F}{F}$
For mass account
for recycle/output



f_A = associated with recycle of A
(contains recycle stream)

$$C_{A_1} = \frac{F_{A_1}}{\epsilon_A} = \frac{F_{A_0} + f_{A_1}}{v_0 + v_1}$$

$$= \frac{F_{A_0} + R F_{A_0} (1 - X_{A_0})}{v_0 + R v_0 (1 + \epsilon_A X_{A_p})}$$

$$= \frac{F_{A_0}}{v_0} \left[\frac{1 + R - R X_{A_0}}{1 + R + R \epsilon_A X_{A_p}} \right]$$

$$\left\{ \begin{array}{l} F_{A_3} = R F_{A_2} \\ R = \frac{F_{A_0} (1 - X_{A_0})}{F_{A_1} (1 - X_{A_0})} \end{array} \right.$$

f_A = take up of recycle part

$$X_{A_1} = \frac{1 - \frac{1 + R - RX_{AB}}{1 + R + R\epsilon_A X_{AB}}}{1 + \epsilon_A \left(\frac{1 + R - RX_{AB}}{1 + R + R\epsilon_A X_{AB}} \right)} = \frac{R\epsilon_A X_{AB} + RX_{AB}}{R + \epsilon_A R + 1 + \epsilon_A} \Rightarrow \frac{RX_{AB}(\epsilon_A + 1)}{(R+1)(\epsilon_A + 1)}$$

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RX_{AB}
 R+1

$$C_{A_1} = C_{A_0} \left[\frac{1 + R - RX_{AB}}{1 + R + R\epsilon_A X_{AB}} \right]$$

$$\begin{cases} C_{A_1} = \frac{1 + R - RX_{AB}}{1 + R + R\epsilon_A X_{AB}} \\ C_{A_0} = \frac{1 + R - RX_{AB}}{1 + R + R\epsilon_A X_{AB}} \end{cases} \quad (B)$$

$$\boxed{X_{A_1} = 1 - \frac{C_{A_1}}{C_{A_0}} = \frac{1 + \epsilon_A C_{A_1}}{1 + \epsilon_A C_{A_1}} \quad (A)}$$

$$\boxed{X_{A_1} = \left(\frac{R}{R+1} \right) X_{AB}} \quad \text{Combining A \& B}$$

$$\boxed{X_{A_1} = \left(\frac{1}{1 + \frac{1}{R}} \right) X_{AB}}$$

If $R \rightarrow \infty$ $X_{A_1} = X_{AB}$ i.e. Perfectly mixed CSTR

Thus for a perfectly mixed CSTR the conversion does not change.

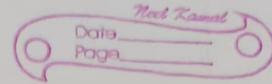
$$\begin{aligned} \frac{V}{F_{A_0}} &= \int_{X_{A_0}}^{X_{A_2}} \frac{dx_A}{(-r_A)} \\ \frac{V}{F_{A_0}} &= (R+1) \int_{X_{A_0}}^{X_{AB}} \frac{dx_A}{\left(\frac{R}{R+1} \right) (-r_A)} \end{aligned}$$

$$\therefore F_{A_0}' = (R+1)F_{A_0}$$

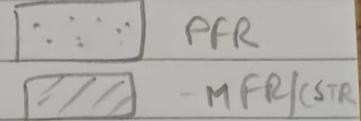
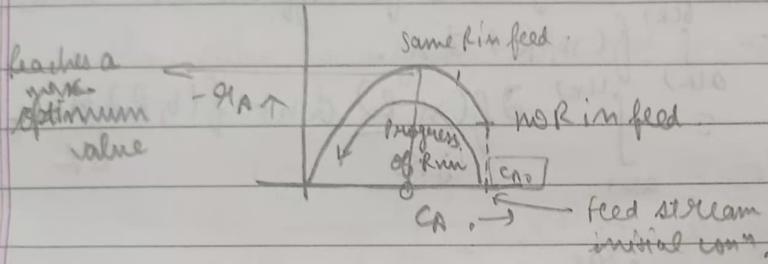
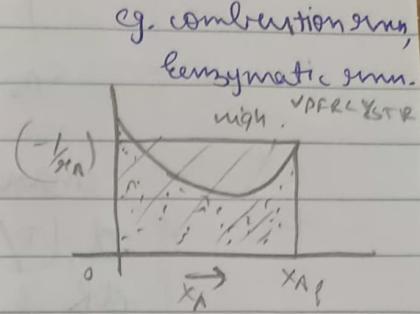
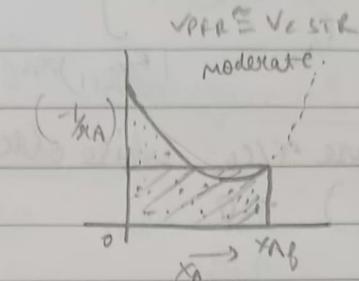
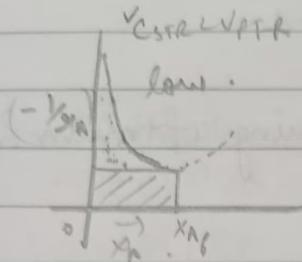
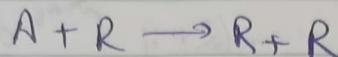
PFR with a recycle
is similar to
PFR with ideal CSTR in
series i.e upto R
length its PFR followed by
a perfectly mixed CSTR

$$\therefore CSTR = \frac{V}{F_{A_0}} = \frac{\dot{V}}{CA_0} - \frac{X_A e^{-R_A t}}{CA_0}$$

$$PFR = \frac{V}{F_{A_0}} = \frac{\dot{V}}{CA_0} - \int \frac{dx_A e^{-R_A t}}{CA_0}$$



Autocatalytic Reaction \rightarrow Run which accelerates the runrate.



Reactor forming product ; product itself acts as reactor

for a given conversion PFR \rightarrow less volume.

In a reversible engn \rightarrow can the conversion be 1 \rightarrow no, full
convertible not possible.

for low, moderate & high conversion. \rightarrow

PFR works better / requires less volume \rightarrow notion works
better for single dir. engn., not for autocatalytic reaction

for autocatalytic engn the curve is not monotonous.

for low conversion $V_{CSTR} < V_{PFR}$ CSTR is better

for moderate conversion $V_{PFR} \approx V_{CSTR}$

for high conversion $V_{PFR} < V_{CSTR}$

Opt finding optimum Recycle Ratio.

$$\frac{\Upsilon}{C_{A_0}} = \frac{v}{f_{A_0}} = (R+1) \int_{\frac{(R/R+1)x_{A_B}}{x_{A_B}}}^{x_{A_B}} \frac{dx_A}{-g_{A_0}} \quad \text{for } \epsilon_A \neq 0.$$

minimise Υ/C_{A_0} while obtaining optimum R

$$\frac{d(\Upsilon/C_{A_0})}{dR} = 0.$$

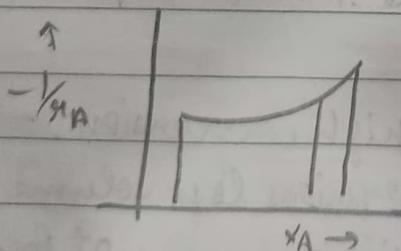
[using Newton Leibnitz Rule for differentiation under integration]

$$F(R) = \int_{a(R)}^{b(R)} f(x, R) dx.$$

$$\frac{dF(R)}{dR} = \int_{a(R)}^{b(R)} \frac{\partial f(x, R)}{\partial R} dx + f(b, R) \frac{db}{dR} - f(a, R) \frac{da}{dR}$$

~~$$\frac{\Upsilon}{C_{A_0}} = (R+1) \int_{\frac{(R/R+1)x_{A_B}}{x_{A_B}}}^{x_{A_B}} \frac{dx_A}{-g_{A_0}}$$~~

$$\frac{d}{dR} \left(\frac{\Upsilon}{C_{A_0}} \right) = \frac{(R+1)}{(R+1)x_{A_B}} \left(\frac{\partial (R+1)}{\partial R} \right) \frac{\partial x_A}{\partial R} + P$$



Multipe run (G7 Levenspiel).

No run practically proceeds through single pathway \rightarrow there is always a side run (In heterogeneous run, using catalyst, the chance of producing side product γ)

Conversion - defined for a reactant
yield, selectivity, rate of formation \rightarrow for product
yield = overall instantaneous.

Assignment - 3

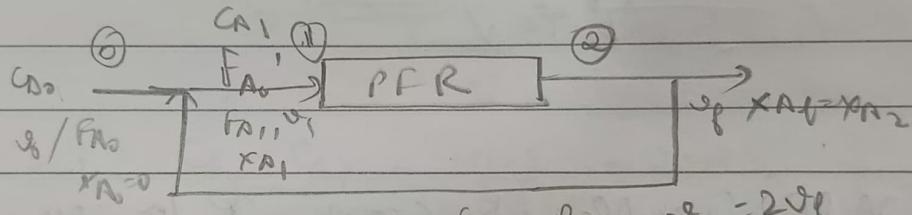
Case 1:
 $x_{A_2} = 0.90 = x_{A_f}$
 $n=1$; i.e. 1st order.
 $C_{A_0} = 10 \text{ mol/l t}$
 $R=2$

normal
PFR.

(Case 2)

$x_{A_f} = 0.9$
 $R=0$.

V_0 : vol. feed flow rate \rightarrow processing rate.



$$F_A 3, R_{uf} = V_3, = 2V_f.$$

$$\frac{C_{A_1}}{C_{A_0}} = \frac{1 + R - Rx_{A_f}}{1 + R + Rx_{A_f}}$$

$$= \frac{1 + 2 - 2(0.9)}{1+2} = \frac{3-1.8}{3} = \frac{1.2}{3} = 0.4$$

$$x_{A_1} = \frac{2}{3} x_{A_f} = \frac{2}{3} (0.9) = 0.6$$

$$\frac{V}{F_{A_0}} = \int \frac{dx_A}{RC_A}$$

$$\underline{\text{Case 2}} \quad K\tau = \ln \frac{C_{A_0}}{C_{A_2}}$$

$$K\tau_2 = \ln \frac{C_{A_0}}{C_{A_0}(1-x_{A_f})}$$

$$K\tau_2 = \ln \left(\frac{1}{1-0.9} \right) \Rightarrow K\tau_2 = \ln 10.$$

$$\text{Case 1} \quad \frac{RT_1}{R+1} = \ln \left[\frac{c_{A_0} + R C_{A_f}}{(R+1) C_{A_f}} \right]$$

$$= \frac{RT_1}{3} = \ln \left[\frac{c_{A_0} + 2 C_{A_0} (1 - X_{A_f})}{(R+1) C_{A_0} (1 - X_{A_f})} \right]$$

$$= \ln \left[\frac{1 + 2 \times 0.1}{3 \times 0.1} \right]$$

$$RT_1' = 3 \ln 4$$

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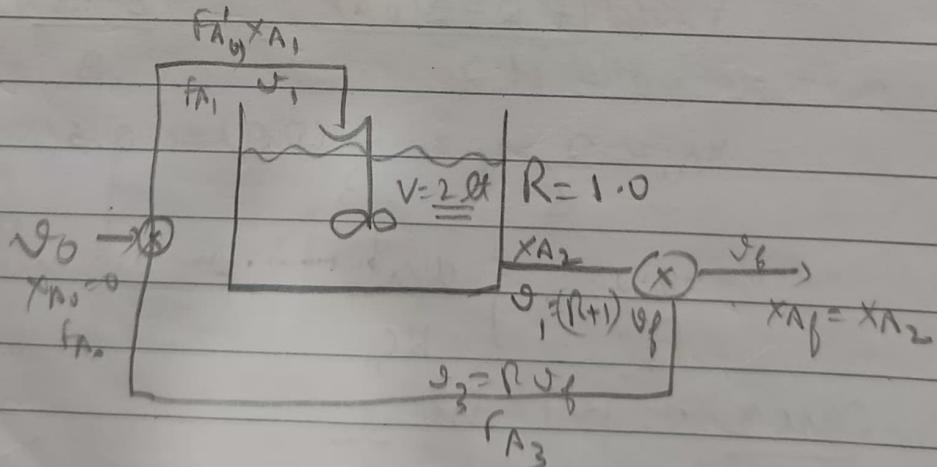
$$\frac{T_2}{T_1} = \frac{\ln 10}{\ln 4}$$

$$= 0.55365$$

$$D T = \sqrt{\frac{R}{V}}$$

If PFR is replaced by CSTR $\frac{T_2}{T_1}$ remains 1;
 \therefore It is already mixed mixture remained into a perfectly mixed ~~near~~ mixture.

$\rightarrow Q.$



$A + B \rightarrow$ Products

$$-\dot{n}_A = 100 \text{ (lt/mol min)} C_A C_B$$

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

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

(i) $X_{A_f} = ?$ ($R = 0$) (ii) $X_{A_f} = ?$ ($\text{when } R \neq 0$)

$$-\dot{r}_A = k C_{A_0} (1 - x_A) (n_0(x_A)).$$

$$-\frac{dC_A}{dx_A} = 0 \Rightarrow C_A = C_R$$

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3. $A \rightarrow R$, $-x_A = 0.001 C_A / kR$ mol/lts.

$$V = 1.5 \text{ l/s. } C_{A_0} = 10 \text{ mol/l. } x_A = \text{highest possible.}$$

4. 1100 L mixed flow reactors. (Solving for.

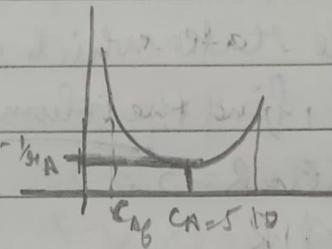
for max. x_A $C_A = C_R$ the highest

$$F_0 + C_{A_0} = 10 = C_A + C_R$$

$$\Rightarrow C_R = C_A = 5.$$

$$-\dot{r}_A = 0.001 (5) (5)$$

$$= 0.025 \text{ mol/lts}$$



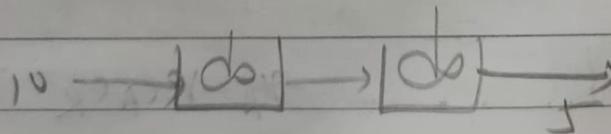
$$\frac{V}{V_0} = \gamma = \frac{C_{A_0} - C_A}{(-\dot{r}_A)} = \frac{10 - 5}{0.025} = 200$$

$$\Delta V \approx V = V_0 \gamma 200$$

$\boxed{\frac{V}{V_0} = 300 \text{ lts}} \rightarrow \text{volume for max. rate.}$

provided

All CSTR in series is not feasible \because It would give least conversion & also volume required would be much higher.



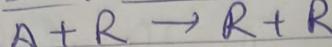
$C_A = 10 \rightarrow \text{must be}$
 $\underline{C_A = 5} \quad \text{followed}$

for any arrangement.

$$\gamma = \frac{V C_{A_0}}{F_{A_0}} = \frac{100(V)}{1.5(V_0)} = \frac{C_A - C_{nf}}{(-\dot{r}_A)}.$$

$$66.67 = \frac{5 - C_{nf}}{0.001 C_{nf} (10 - C_{nf})}$$

→ Optimum Recycle Ratio for an Autocatalytic Rxn-



$$-\dot{R}_A = k C_A C_R.$$

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

$$C_{A_0} = 10 \text{ mol/lit.}$$

$$C_{R_0} = 0$$

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

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

- (a) find the recycle rate which will minimize the size of reactor, find the volume.

(b) $\frac{V_{PFR}}{V_{RPF}} = ?$ when $R = 5$.

(c) $R = \infty, V = ?$; ($R = 0, V = ?$)
(MFR) (ideal PFR).

Ans. $\frac{V}{F_{A_0}} = (R+1) \int_{\frac{R}{R+1} X_{A_f}}^{X_{A_f}} \frac{dX_A}{-\dot{R}_A}$

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

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

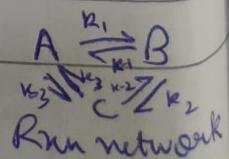
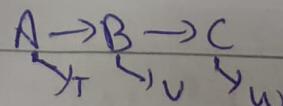
$$\rightarrow \int_{\frac{R}{R+1} X_{A_f}}^{X_{A_f}} \frac{dX_A}{(-\dot{R}_A)} \quad -\dot{R}_A = k C_A C_R \\ = k C_{A_0}^2 (1-X_A)$$

→ Multiple Reactions

1) Series Rxn (consecutive Rxn).

2) Parallel Rxn (competitive Rxn)

3) Series-parallel Rxn



$Rxn \text{ network}$

Reversible - Irreversible series Run

Reversible - Irreversible Parallel Run

Run network - Branch of ~~or~~ series - parallel run.

e.g. of such run network include (1) Biochemical Run (enzymatic)

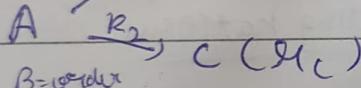
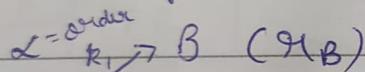
(2) Polymer Synthesis Run ; 3) Drug Industry, 4) Combustion ^{run}

→ yield of a run ; selectivity of a run \rightarrow imp. for single run.
(since only single product).

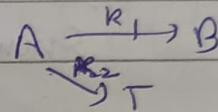
→ Based on kinetics & temp of a run

k_1 , may or may not be = $t \cdot k_2$

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



B = order



Assumptions 1) density = const ($\epsilon = 0$)

2) first order

3) liq. phase run (const. density)

$$-\dot{\eta}_A = \dot{\eta}_{1B} + \dot{\eta}_{1C}$$

$$\left(-\frac{dC_A}{dt} \right) = \frac{dC_B}{dt} + \frac{dC_C}{dt}$$

product distribution ; yield of desired product \rightarrow based on type of reactor in which run takes place

$$\frac{\eta_{1B}}{\eta_{1C}} = \frac{\frac{dC_B}{dt}}{\frac{dC_C}{dt}} = \frac{\frac{dC_B}{dt}}{\frac{dC}{dt}} = \frac{k_1 C_A^\alpha}{k_2 C_A^\beta} = \frac{k_1}{k_2} C_A^{\alpha - \beta}$$

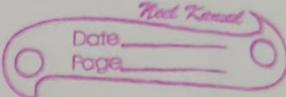
Based on values of α & β

1) $\alpha > \beta \rightarrow$ High η_{1B} , if C_A is high.

2) $\alpha < \beta \rightarrow$ Low η_{1B} , if C_A is low

3) $\alpha = \beta \rightarrow$ no matter.

$PFR = \text{infinite CSTR}$



by changing T

for high rate of B, k_1 and k_2 can be varied, but considering isothermal cond. k_1 & k_2 not varying (assumed)

$\alpha > \beta$ \Leftrightarrow for high C_A 1) PFR. 2) Pressure is high \Rightarrow less inert
3) Maintaining low conversion

$$\underline{\text{PFR (Batch)}} \quad \therefore \underline{t_{\text{batch}} = T_{\text{PFR}}} \text{ (for const. volume v)}$$

$\alpha < \beta \Leftrightarrow$ for low C_A 1) CSTR 2) less pressure 3) more inert

∴ mixing of reactants & type of reactor is imp. for multiple stages.

→ Contacting Pattern

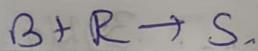
1) $C_A, C_B \uparrow$ both

2) $C_A, C_B \downarrow$ both

3) $C_A \uparrow, C_B \downarrow$

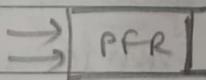
4) $C_A \downarrow, C_B \uparrow$.

to understand how contacting pattern does affect product

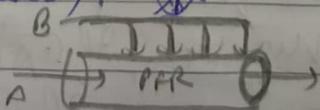


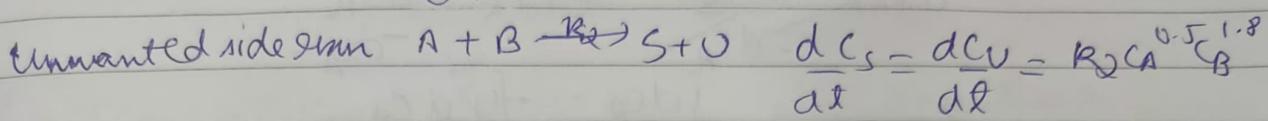
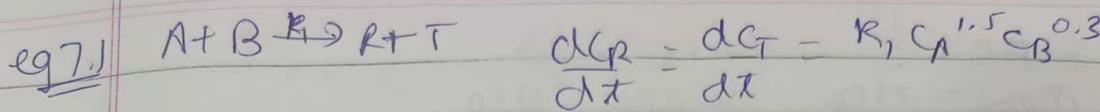
→ $C_A, C_B \uparrow$ both \rightarrow Initially present (both C_A & C_B) \rightarrow both Reactants stream mixed in PFR / Batch.

Initially present
(Batch/PFR).



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

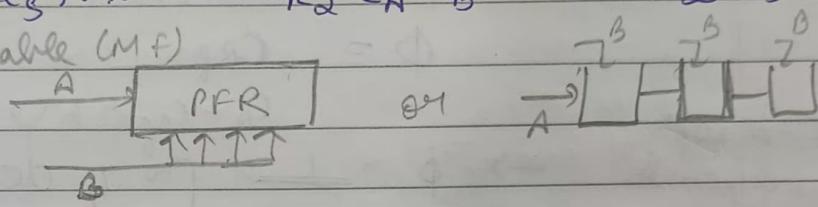




From the standpoint of favourable product distribution, order the contacting schemes of Fig. 7.2., from the most desirable to the least desirable.

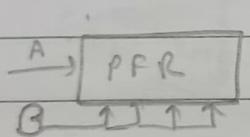
$$R_B = \frac{dc_R/dt}{dc_S/dt} = \frac{k_1 C_A^{1.5} C_B^{0.3}}{k_2 C_A^{0.5} C_B^{1.8}} = \frac{k_1 C_A^1}{k_2 C_B^{1.5}}$$

most favourable (MF)



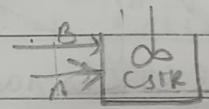
MF

least favourable



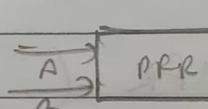
high C_A

low C_B



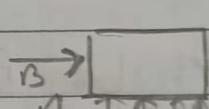
low C_A

low C_B ($\because 1.5 > 1$)



high C_A

high C_B



low C_A

high C_B

$\rightarrow \psi$ = Instantaneous yield. \rightarrow fractional yield at each instant of time. (Batch with time, PFR with position)
 ϕ = Overall fractional yield.

For $A + B \rightarrow R$, desired
 $\rightarrow S$, unwanted.

$$\psi = \frac{(dc_R/dt)}{(-dc_A/dt)} =$$

$$(-dc_A/dt)$$

$$\phi = \frac{\text{moles of } R \text{ formed}}{\text{all moles of } A \text{ reacted}} = \frac{c_R f}{c_{A_0} - c_{A_f}}$$

f = final

$$\Delta C_A = C_{A_f} - C_{A_0}$$

$$= \frac{c_{Rf}}{(-\Delta C_A)}$$

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

~~$$\Phi_{PFR} = \frac{dc_A}{-dc_A}$$~~

$$\Psi_{PFR} = \frac{dc_A}{-dc_A}$$

$$\int dc_A = \int \Psi dC_A$$

$$\int_{C_A0}^{C_Af} dc_A = \int_{C_A0}^{C_Af} \Psi dC_A$$

$$C_{Rf} = \int_{C_Af}^{C_A0} \Psi dC_A$$

$$\Phi = \frac{C_{Rf}}{C_A0 - C_Af}$$

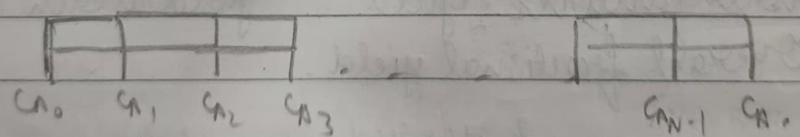
In PFR, the com
depth is general

$$\rightarrow \Phi = \frac{\int_{C_A0}^{C_Af} \Psi dC_A}{C_A0 - C_Af}$$

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

$$\Phi_{MFR} = \Psi \text{ at } C_Af = \frac{dc_A}{(-dc_A)} \Big|_{C_Af}$$

for N reactors MFR in series



$$\Phi_{MFR} = \prod_{i=1}^N (\Psi_i) \quad i=1, \dots, N.$$

$$\Phi_{MFR} = \frac{C_{Rf}}{C_A0 - C_Af}$$

$$\Psi_{MFR} = \frac{dc_A}{(-dc_A)} = \frac{C_{Rf}}{C_A0 - C_Af}$$

$$\Rightarrow \boxed{C_{Rf,MFR} = \Psi (C_A0 - C_Af)}$$

$$\boxed{C_{Rf,MFR} = \int_{C_Af}^{C_A0} \Psi dC_A}$$

$$\Phi_{NMFR} = \frac{\sum_{i=1}^N \Phi_N}{C_{A_0} - C_{A_N}} = \frac{\sum_{i=1}^N \Psi_i (C_{A_{i-1}} - C_{A_i})}{C_{A_0} - C_{A_N}}$$

Eg. $\frac{dC_R}{dt} = R_1 C_A C_B^{0.5}$ mol/lt min $A + B \xrightarrow{k} R$, desired

$$\frac{dC_S}{dt} = R_2 C_A^{0.5} C_B^{1.5}$$
 mol/lt min $A + B \xrightarrow{k_2} S$, undesired $k_1 = k_2 = 1$

$X_{Af} = 90\%$. Find C_R, C_S for volume flow rate of A & B

- (a) Plug flow. (b) MFR (c) Best of them ~~20 mol/lt.~~

Ans. (i). For PFR:

$$C_{Rf} = \int_{C_{A_0}}^{C_{A_f}} \Psi dC_A$$

$$\Psi = \frac{C_{A_f}}{C_{A_0}} \frac{dC_R}{dC_A} = \frac{R_1 C_A C_B^{0.5}}{R_2 C_A^{0.5} C_B^{1.5}} = C_A^{0.5} C_B^{-1.0}$$

$$C_{Rf} = \int_{C_{A_0}}^{C_{A_f}} C_A^{0.5} C_B^{-1.0} dC_A$$

$$C_{A_f} = C_{A_0} (1 - X_{Af})$$

$$C_{A_f} = 20 (1 - 0.9) = 2$$

$$C_{Rf} = \int_{2}^{20} C_A^{0.5} C_B^{-1.0} dC_A$$

$$C_{Rf} = \frac{1}{1.5} [20^{1.5} - 2^{1.5}]$$

$$C_{Rf} = \frac{1}{1.5} [20^{1.5} - 2^{1.5}]$$

$$\frac{(P(R))}{(A)} \frac{dC_R}{dt} = \frac{R_2 C_A C_B^{0.5}}{k_1 C_A C_B^{0.5} + k_2 C_A^{0.5} C_B^{1.5}} = \frac{C_A^{0.5}}{C_A^{0.5} + C_B^{1.0}}$$

$$\therefore C_{R,f,PFR} = \int_{C_{A_0}}^{C_{A_f}} \frac{C_A^{0.5}}{C_B + C_A^{0.5}} dC_A$$

$$\Phi_{PFR} = \left(\int_{10}^1 \frac{C_A^{0.5}}{C_B + C_A^{0.5}} dC_A \right) \frac{1}{C_{A_0} - C_{A_f}}$$

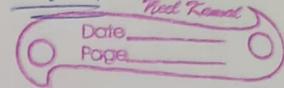
$$\Phi_{PFR} = \left(\int_{10}^1 \frac{C_A^{0.5}}{C_A + C_B^{0.5}} dC_A \right) \frac{1}{C_{A_0} - C_{A_f}} = 0.32$$

$C_A = C_B$

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

$$\Phi = \int_{\text{PFR}} \Psi dC_A \quad \Phi = \Psi \text{ at } f.$$

$$C_{Af} + C_{Sf} = \Delta C_A = C_{A0} - C_{Af}$$



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

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

$$b). \Phi_{MFR} = \Psi \text{ at } C_{Af} = \frac{dC_R}{dC_A} \Big|_{C_{Af}} = \frac{C_A^{0.5}}{C_{Af} + C_A^{0.5}} = 0.5$$

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

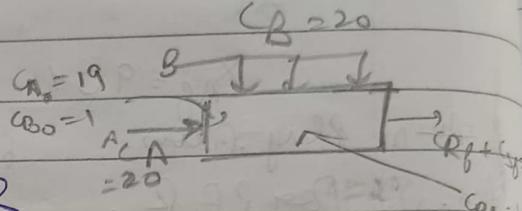
$$C_{Sf} = 9 \times 0.5 = 4.5$$

c). PFR-MFR mixed,

$C_A \rightarrow$ gradually $\rightarrow A$ as PFR

C_B ↓ drastically \leftarrow 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 to T Φ . $C_{Af} \rightarrow 19 (10+9)$.



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

$$= 0.932$$

$$C_{Rf} = \cancel{0.932}$$

$$C_{A0} = 19, C_A = 1$$

$$C_{Bf} = 1.$$

$$\Phi \left(\frac{R}{A} \right) = \left(\int_{19}^1 \frac{C_A^{0.5}}{C_B + C_A^{0.5}} dC_A \right) \frac{1}{C_{A0} - C_{Af}}$$

$$\Phi \left(\frac{R}{A} \right) = \left(\int_{19}^1 \frac{C_A^{0.5}}{1 + C_A^{0.5}} dC_A \right) \frac{1}{19-1}$$

$$I_1 = \int_1^{19} dC_A = 18$$

$$I_2 = \int_1^{19} dC_A / (C_A^{0.5} + 1) =$$

$$\Phi \left(\frac{R}{A} \right) = \frac{1}{18} [I_1 - I_2]$$

Finally $\Phi \left(\frac{R}{A} \right) = 0.87$

$$C_{Rf} = 9 \times 0.87 \\ = 9 \times 0.87$$

$$= 7.85$$

$$C_{Sf} = 9 - 7.85 \\ = 1.15$$

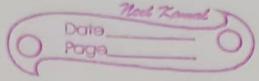
leg 7.3

a)

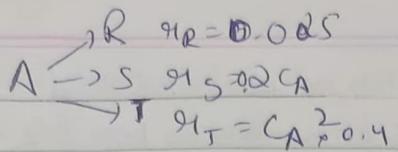
Ans

MFR
at

P:



Eq 7.3



Find minimal expected C_S for
isothermal operations.

a) in MFR

b) in PFR

c) Recycle to the feedat

$$\text{Ans} a) \Phi\left(\frac{S}{A}\right) = 0 \text{ at } C_f$$

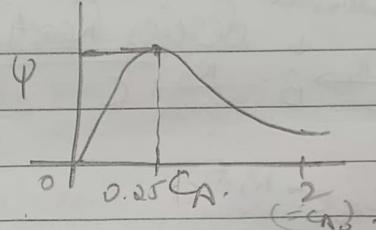
$$(MFR + PFR) = 2 \\ C_{A_0} = 2$$

\rightarrow PFR with an MFR.

$$\cancel{\Phi\left(\frac{S}{R}\right)} = \cancel{\Phi\left(\frac{S}{A}\right)}$$

$$\Phi\left(\frac{S}{A}\right) = \frac{dCS/dt}{-dC_A/dt} = \frac{2C_A}{1 + 2C_A + C_A^2/2} = \frac{0.2(C_A)^2}{(C_A + 1)^2}$$

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



$$c) \quad C_S = \Delta C_A * \Phi \text{ at } C_f.$$

For MFR, area under curve has to be minimised

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

$$C_S = (C_{A_0} - C_{A_f}) \left[\frac{8C_f}{(1+4C_f)^2} \right]$$

$$\frac{dC_S}{dC_{A_f}} = 0.$$

$$\frac{dC_S}{dC_{A_f}}$$

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

$$\frac{dC_S}{dC_{A_f}} = (1+4C_{A_f})^2 [16] - 16C_{A_f} [2(1+4C_{A_f})^4] - d \frac{8C_f^2}{(1+4C_f)^2} = 0$$

$$= C_{A_f} = 0.20 \approx (1/5)$$

$$C_S = \underline{\underline{8/9}}$$

MFR \rightarrow more area than PFR

PFR
 \therefore more conversion.

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

A

$$\therefore C_{A_f} = 0$$

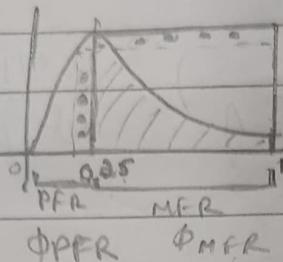
$$C_S = \underline{\underline{0.654}}$$

c). $\therefore C_p^2$ in denominator as compared to C_A .

$\therefore C_p$ must be kept as low as possible \rightarrow MFR has more area.

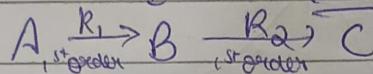
\therefore find the point at which minimum Φ occurs till they operate under MFR i.e. till $C_p = \underline{0.25}$ (here).

Case I



$$C_{Sp} = \underline{0.972}$$

Intermediate (may be desired / undesired).
 → Series Reaction,

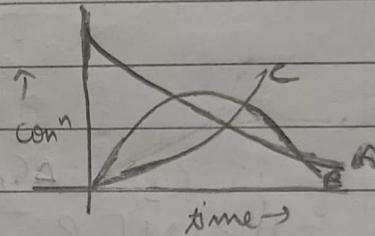


C_A

$$C_A = C_{A_0} e^{-R_1 t}$$

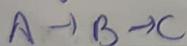
C_B

C_C



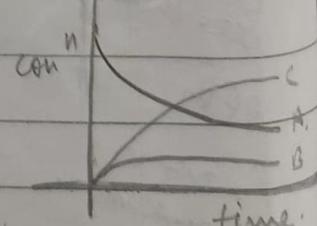
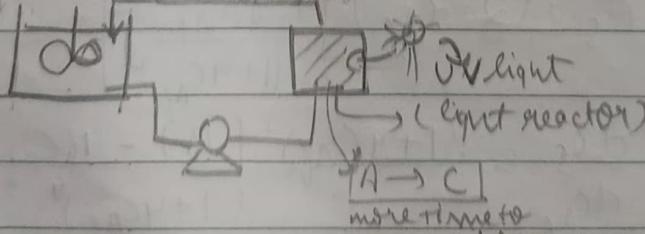
If B is undesired, we have to see the way through which min. B, while max. C is formed.

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

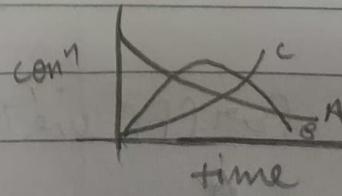
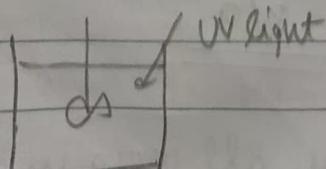


light starts)

(unconverted A)



Case 2 → whole reactor exposed to light.



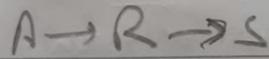
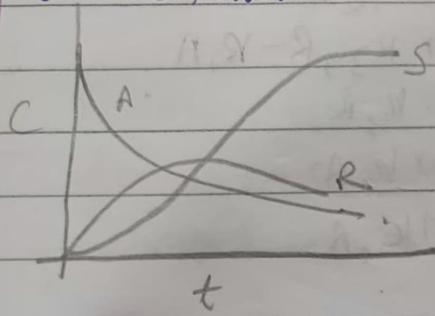
Case I

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

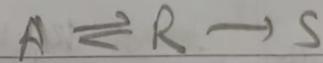
- for parallel reactor - conⁿ of A is important
- R or series → intermediate prod. conⁿ is imp.
- so: PFR or batch - better to control intermediate prod.
since mixing is not prominent (batch ∵ we can control batch time)
- CSTR → better for control conⁿ of reactant, product ∵ mixing is prominent.

Q Find t_{opt} for C_B max/min. Batch time PFR time MFR time

→ Write sum network

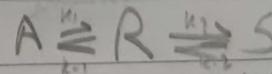
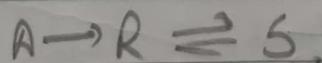


$$k_1 = k_2 = 1$$

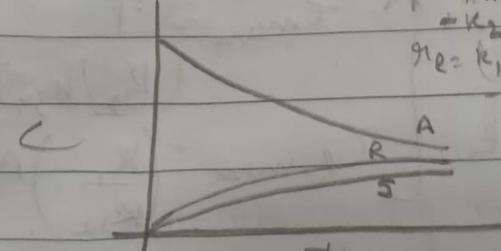
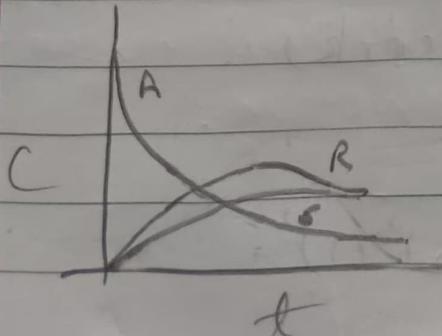


slow depletion of A, non-interacting A & R

$$k_1 = k_2 = 1$$

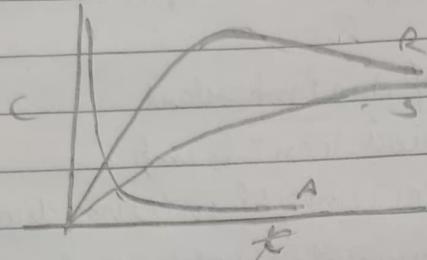


$$\begin{aligned} g_{1P} &= k_1 C_A - k_1 C_R \\ &\quad + k_2 C_R + k_2 C_S \\ g_{1R} &= k_1 C_A + k_2 C_S - k_1 C_R - k_2 C_R \end{aligned}$$



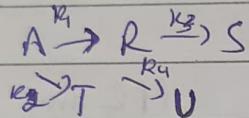
$$C_A + C_S = 2C_0 \quad g_{1S} = k_2 C_R - k_2 C_S$$

If $A \xrightarrow{k_1} R \xrightarrow{k_2} S$



$A + R \rightarrow R + S$ → In PFR; Recycle reactor is used
R promotes more than.

Denbigh



find $C_{R,\text{max}}$ & t_{max} in terms of rate constant.

$$-\dot{R}_A = [R_1, A + R_2, A] \Rightarrow R_{1,2} A$$

$$-\dot{R}_R = R_3 R + R_4 R - R_1, A \Rightarrow k_{34} R - R_1, A$$

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

$$\dot{R}_T = R_1, A \Rightarrow R_1, A$$

$$\dot{R}_U = R_4 R \Rightarrow R_4 A$$

~~n.w check~~

$$\therefore R_{1,2} = R_1 + R_2$$

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

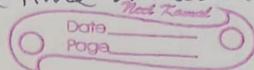
for batch & PFR,

$$\left\{ \begin{array}{l} t_{\text{max}} = \ln \left(\frac{k_{34}}{k_{1,2}} \right) \cdot (T \text{ for PFR}) \\ C_{R,\text{max}} = C_{A_0} \cdot \frac{k_1}{k_{1,2}} \left(\frac{k_{1,2}}{k_{34}} \right)^{\frac{k_{34}}{k_{34}-k_{1,2}}} \end{array} \right.$$

for CSTR,

$$\left\{ \begin{array}{l} t_{\text{max}} = \frac{1}{\left(\frac{k_{1,2}}{k_{34}} \right)^{k_2}} \quad (\text{for CSTR}) \\ C_{R,\text{max}} = \left(\frac{R_1}{R_{1,2}} \right) A_0 \cdot \frac{1}{\left(\left(\frac{k_{34}}{k_{1,2}} \right)^{k_2} + 1 \right)^2} \end{array} \right.$$

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



Non-Ideal Reactors Real Reactors

Imperfections in reactor reduces rate of reaction
ideal reactor \rightarrow highest conversion always.

Imperfections \rightarrow Residence time distribution.

Ideal reactor - Reactor in which ^{each} packets of elements spend same time in a reactor.

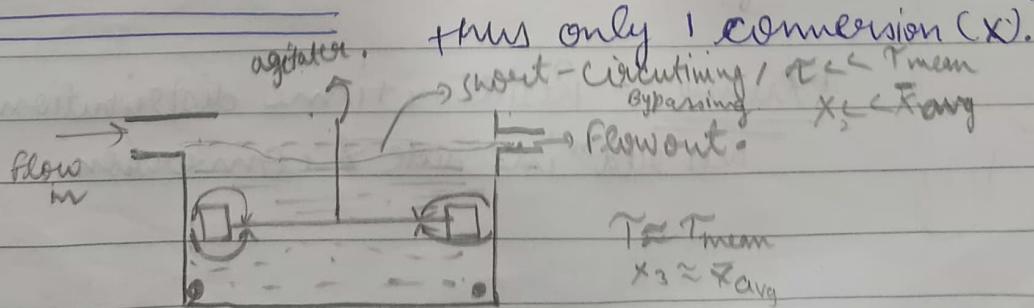
for a tracer molecule \rightarrow molecule used to trace the time spent in a reactor.

the ^{input} pulse given can be pulse or step.

Residence time - time a molecule spends inside a reactor
if there is distribution of time \rightarrow the conversion may be different.

Real reactor - T_{mean} = mean residence time / avg. residence time
different batch have diff. T_{mean}
thus we get a \bar{T}_{avg} .

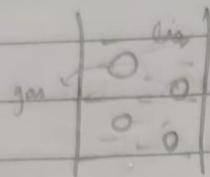
Ideal reactor - $T =$ constant residence time (only).



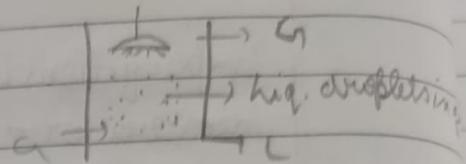
Stagnant region (remains even if $E \rightarrow \infty$)
 \therefore (in this region $X \rightarrow 1$)

→ gas-liquid r.m. - 2 ways of contact.

gas is bubbled through liq. | liq. sprayed through gas flow



sparger reactor

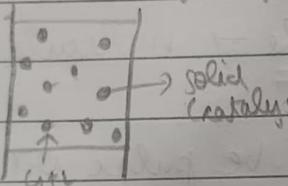


spray tower reactor

effect
different.

→ channelling ^(or bypass) - very prevalent in 2 phase reactor also in packed
 r.m. operation.

3-phase (Solid-gas-liq.) reactor.



↑
gas or liq. find a less
resistance path to go out
without interacting with solid

→ e.g. of channelling

channelling is more in 3 phase r.m. , lesser in single phase r.m.

These anomalies reduces the rate of r.m. .

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

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

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