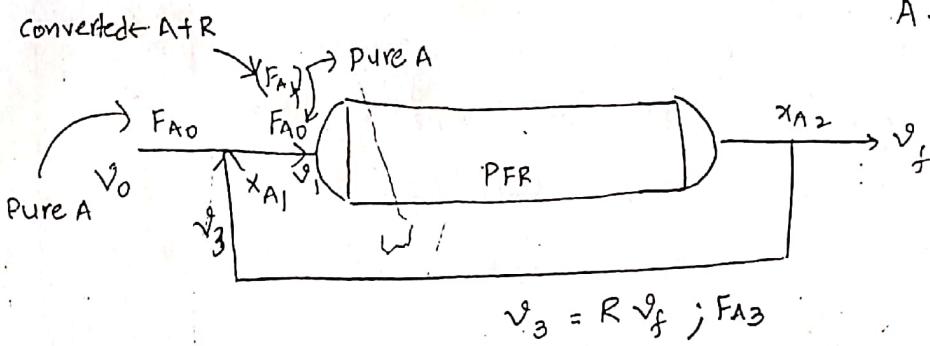


# RECYCLE REACTOR



$R = \frac{\text{Volume of fluid returned to the feed}}{\text{volume leaving the system}}$

$$R = \frac{V_3}{V_f}$$

$$\frac{V}{F_A0} = \int_{x_{A1}}^{x_{A2}} \frac{dx_A}{-r_A}$$

$$F_A0' = F_A0 + R F_A0$$

$$F_A0' = (R+1) F_A0$$

$$x_{A1} = \frac{1 - C_{A1}/C_{A0}}{1 + \epsilon_A C_{A1}/C_{A0}}$$

- Backmixing of the product stream
- conversion of the inlet stream changes
- mole balance  $F_A0' \rightarrow$  pure A

$$F_A0' = F_A0 (1-x_A)$$

$$C_{A1} = \frac{F_{A1}}{V_1} = \frac{F_{A0} + F_{A3}}{V_0 + R V_f} = \frac{F_{A0} + R F_{A0} (1-x_{Af})}{V_0 + R V_f (1+\epsilon_A x_A)}$$

$$C_{A1} = C_{A0} \frac{\left(1 - \frac{R}{R+1} x_{Af}\right)}{\left(1 + \frac{R \epsilon_A x_A}{R+1} f\right)} = \frac{F_{A0} (1+R(1-x_{Af}))}{V_0 (1+R(1+\epsilon_A x_A))}$$

$$X_{A1} = \frac{R}{R+1} X_{Af}$$

$$C_{A1} = C_{A0} \left[ \frac{1 - X_{A1}}{1 + \epsilon_A X_{A1}} \right]$$

A substance A <sup>reac.</sup> according to second order kinetics and conversion is 95%. from a single flow reactor. We buy a second unit identical to the first. For the same conversion, by how much is the capacity increased if we operate these two units in parallel or in series?

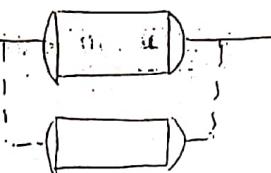
- (a) The reactors are both plug flow.
- (b) The reactors are both mixed flow.

(a) PFR

# Parallel

For a single reactor

$$\frac{V}{F_{A01}} = \int_0^{X_A} \frac{dx_A}{-r_A} = \int_0^{0.95} \frac{dx_A}{K C_{A0}^2 (1-x_A)^2}$$



$$C_1 K C_{A0} = \frac{X_A}{1-X_A} = \frac{0.95}{0.05} = 19$$

$$V K C_{A0} = 19 v_1$$

$$C_2 K C_{A0} = 19$$

$$V K C_{A0} = 19 v_2$$

$$v_1 = v_2$$

$$v_1 + v_2 = 2v_2$$

# Series

$$\frac{V}{F_{A0}} = \int_0^{X_A} \frac{dx_A}{K C_{A0}^2 (1-x_A)^2} = I$$

Single

$$\frac{V_1}{F_{A02}} = \int_0^{X_{A1}} \frac{dx_A}{K C_{A0}^2 (1-x_A)^2}$$

$$\frac{V_2}{F_{A02}} = \int_{X_{A1}}^{X_{A2}} \frac{dx_A}{K C_{A0}^2 (1-x_A)^2}$$

and  
we buy

me  
used if  
series?

$$\frac{V_1 + V_2}{F_{A0}} = \int_0^{X_A} \frac{dx_A}{K_{CA0}(1-x_A)^2} + \int_{X_A}^{Y_A} \frac{dx_A}{K_{CA0}^2(1-x_A)^2} = I$$

$$\therefore \frac{2V}{F_{A0}} = I = \frac{V}{F_{A0}} \quad V_1 + V_2 = 2V$$

### (b) MIXED REACTOR

# Parallel

$$\frac{V}{F_{A0}} = \frac{X_A}{K_{CA0}^2(1-x_A)^2} = \frac{380}{K_{CA0}^2}$$

$$C_1 = \frac{380}{K_{CA0}} \quad \text{or} \quad \frac{V}{V_1} = \frac{380}{K_{CA0}}$$

$$\frac{V}{F_{A0}} = \frac{X_A}{K_{CA0}^2(1-x_A)^2}$$

$$\stackrel{1st}{\Rightarrow} \frac{VK_{CA0}}{V_1} = \frac{X_A}{(1-x_A)^2} = \frac{0.95}{(0.05)^2} = 380$$

$$\Rightarrow VK_{CA0} = 380 V_1$$

$$\stackrel{2nd}{\Rightarrow} \frac{VK_{CA0}}{V_2} = 380 \quad \frac{VK_{CA0}}{V_2} = 380$$

$$V_2^I = V_2^{II} = \frac{VK_{CA0}}{380}$$

$$V_2 = 2V_1$$

$$(1-x_A)^2$$

$$\frac{dx_A}{K_{CA0}^2(1-x_A)^2}$$

~~(#)~~ Series

$$V = V_1$$

$$C = \frac{x_1}{KC_{AO}(1-x_f)^2} = \frac{380}{KC_{AO}}$$

$$\boxed{C_1 = C_2}$$

$$\frac{x_1}{KC_{AO}(1-x_1)^2} = \frac{x_2 - x_1}{KC_{AO}(1-x_2)^2}$$

$$\Rightarrow \frac{x_1}{(1-x_1)^2} = \frac{0.95 - x_1}{(0.05)^2} \quad \leftarrow \boxed{x_2 = 0.95}$$

=> solve for  $x_1$

By trial  $x_1 = 0.8525$

$$C_1 KC_{AO} = 39.18$$

$$\frac{V}{V_2} KC_{AO} = 39.18$$

$$\frac{V}{V_1} * \frac{V_2}{V} = \frac{380}{39.18}$$

$$\frac{V}{V_1} KC_{AO} = 380$$

$$\frac{V_2}{V_1} = 9.698 \approx 10$$

Presently 90% of reactant A is converted into product by a second order reaction in a single mixed flow reactor. We propose to place a second reactor similar to the one being used in series with it.

- (i) For the same treatment rate as that used presently how will this addition of reactor affect the conversion of reactant?
- (ii) For the same 90% conversion, by how much can the treatment rate be increased in the latter case?

# Recycle reactor design

$$\frac{V}{F_{A0}} = R+1 \int_{\frac{R}{R+1}x_{Af}}^{x_{Af}} \frac{dx_A}{-\dot{r}_A}$$

GENERAL

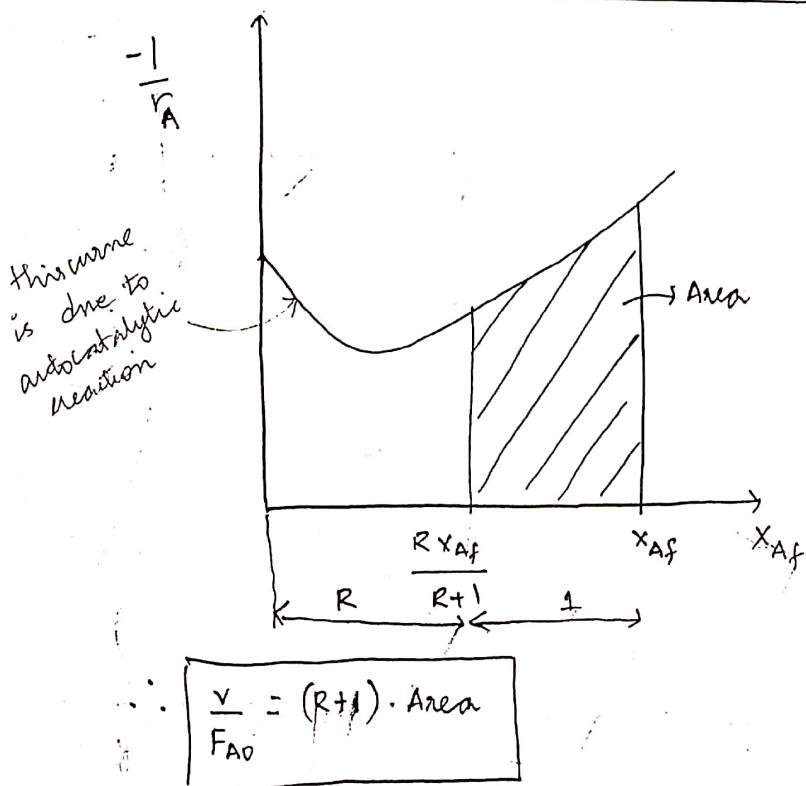
$$\Rightarrow C_R = \frac{C_{AO} V}{F_{A0}} = -(R+1) \int_{\frac{C_{AO} + RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{-\dot{r}_A}$$



for  $\epsilon = 0$   
liq phase  
or  
no inerts

$$x_{Ai} = f(x_{Af})$$

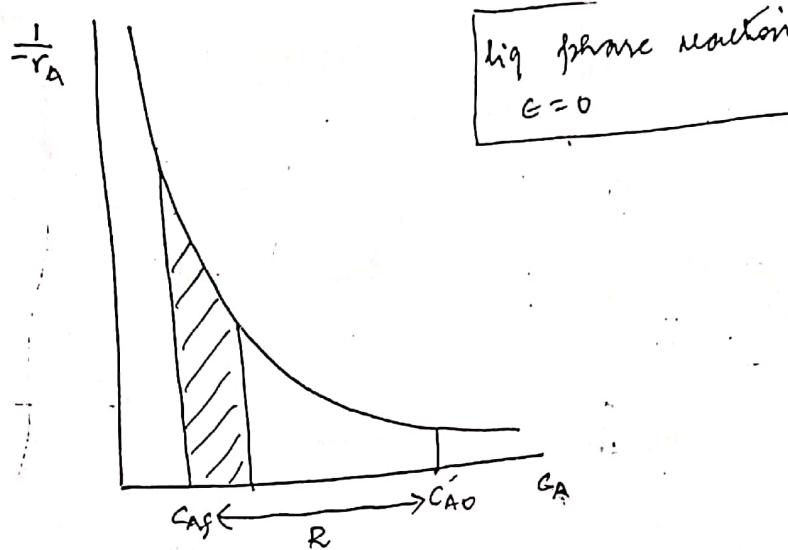
$x_A$  - any values



- #1 Find the recycle ratio  $R$
- #2.  $R$  should be the optimised recycle ratio
- #3: find  $x_{Ai}$  in terms of  $R$  &  $x_{Af}$ .

• Recycle  
(der)

base  
inerts

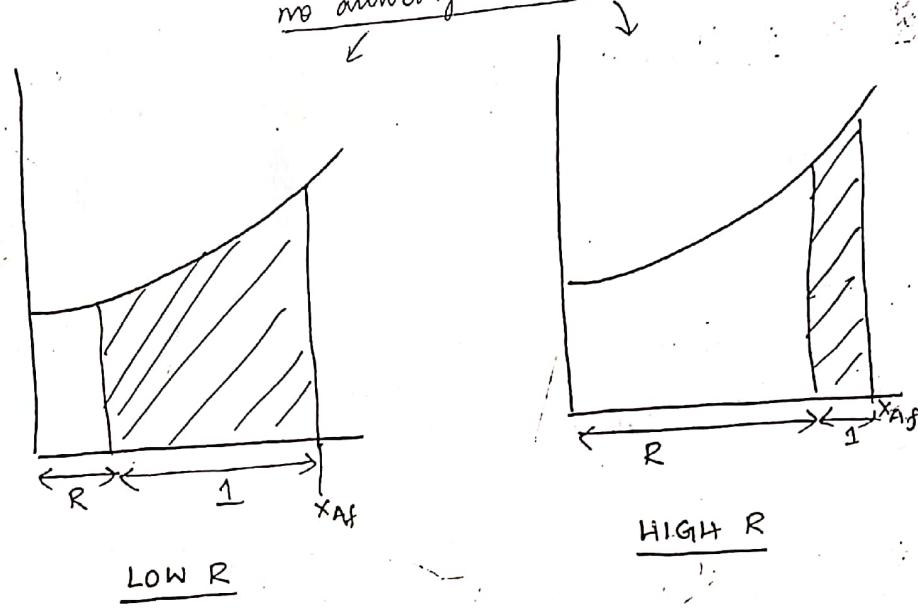


liq phase reaction  
 $E=0$

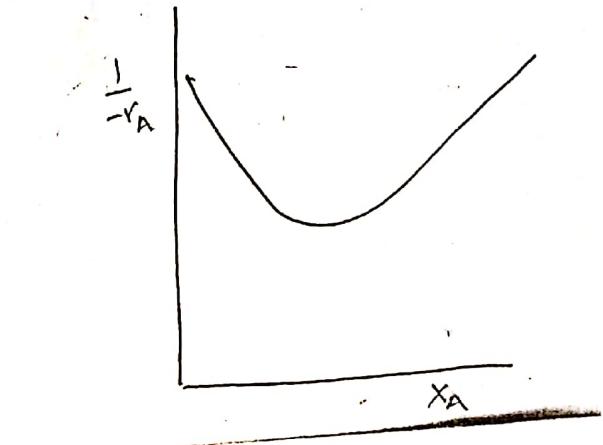
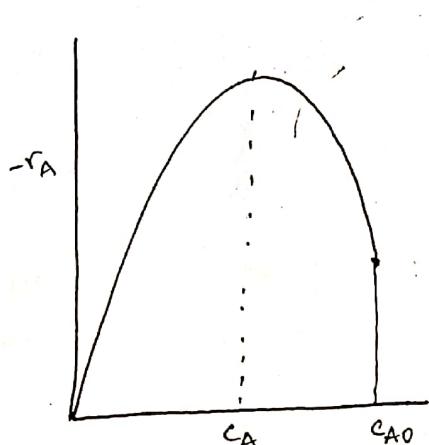
#1 Find the recycle ratio  $R$

#2.  $R$  should be the optimised recycle ratio

#3: Find  $x_{Ai}$  in terms of  $R$  &  $x_{Af}$ .



- Reactant acting as a catalyst - Autocatalytic reaction  
(densified)  $A + R \rightarrow R + R$

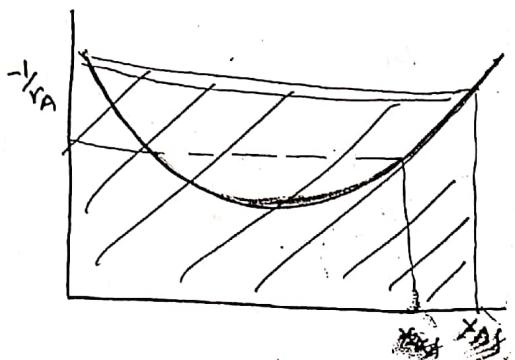


$$\frac{a_1 - C_{AD}}{dR}$$

Using eqn

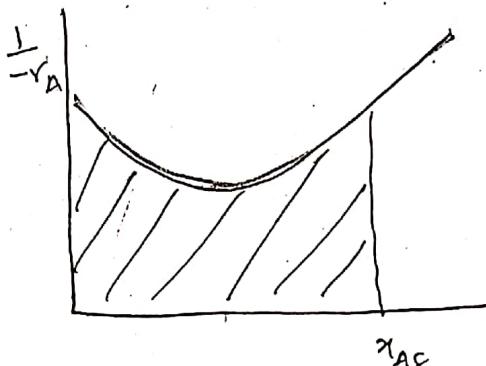
$$-\frac{1}{r_A} \quad x_A$$

using vcm



Large volume required

Using TRK



less volume required

TO FIND THE OPTIMIZED 'R' : PROCEDURE:-

$$\#1. \frac{C}{C_{AD}} = \int_{x_{Ai}}^{x_{Af}} \frac{R+1}{-r_A} dx$$

$$\#2. \frac{\partial (C/C_{AD})}{\partial R} = 0 \quad \Rightarrow$$

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

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

Applying the above formula:

$$\bullet a(R) = x_{Af} \frac{R}{R+1} \quad \bullet \frac{da}{dR} = \left( \frac{R+1 - R}{(R+1)^2} \right) x_{Af} = \frac{x_{Af}}{(R+1)^2} \quad \text{eq ①}$$

$$\bullet b(R) = \text{constant} = x_{Af}$$

$$\bullet x_{Af} - x_{Ai} \Rightarrow x_{Af} - x_{Ai} \frac{R}{R+1} = \frac{x_{Af}}{(R+1)} \rightarrow \text{eq ②}$$

From this  
BE SUCH  
CAN EVA

$$\frac{1}{r_A} \quad \frac{1}{r_{Avg}}$$

TO FIN

A →

cost of

Feed

C\_M

FIND

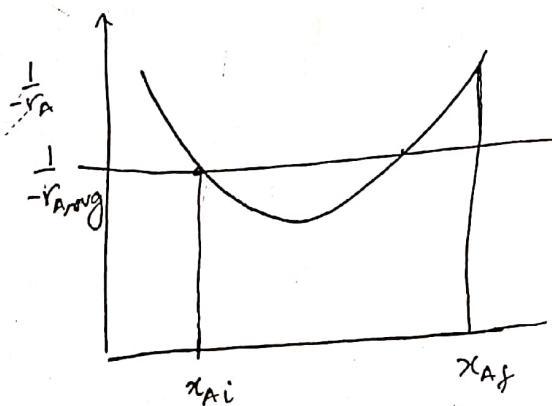
RAT

$$\frac{d(\ln(C_{A0})}{dR} = 0 = \int_{x_{Ai}}^{x_{Af}} \frac{dx_A}{-r_A} + 0 - \left. \frac{R+1}{-r_A} \right|_{x_{Ai}} \frac{dx_{Ai}}{dR} \quad \text{--- eq(3)}$$

Using equation 1, 2, 3:-

$$\boxed{-\frac{1}{r_A} \Big|_{x_{Ai}} = \frac{\int_{x_{Ai}}^{x_{Af}} \frac{dx_A}{-r_A}}{(x_{Af} - x_{Ai})}} \Rightarrow \text{average of } \frac{1}{-r_A} = \frac{1}{r_{A,\text{avg}}}$$

From this we can note that : RECYCLE POINT WILL BE SUCH THAT , IT LIES ON THE LINE  $\frac{1}{-r_{A,\text{avg}}}$ ; OR WHERE WE CAN EVALUATE  $\frac{1}{-r_{A,\text{avg}}}$ ;



At  $x_{Ai}$ ,  $\frac{1}{-r_{A,\text{avg}}}$  is evaluated.

### TO FIND OPTIMUM REACTOR SIZE



$$\text{cost of Reactant (C}_{A0}\text{)} = C_R R_s / \text{Kmol A}$$

$$= F_{A0} \text{ Kmol / hr}$$

Feed rate

$$C_M = (\text{cost of Reactor}) + (\text{cost of installation + overhead + labor}) * R_s / (\text{hr. lt of reactor volume})$$

FIND THE OPTIMIZED COST FOR A DESIRED PRODUCTION RATE  $F_R$  Kmol/hr.

Total cost  $C_T = C_M \cdot V + F_{AO} \cdot C_R$  [Rs/hr]

Some depreciation cost is also added, not shown.

$F_{AO}$  can be found using  $F_{AR}$  if conversion is known.

#  $F_{AO} = F_{AD} \cdot X_A$

#  $F_{AD} = \frac{F_R}{X_A}$

$$V = \frac{F_{AO} \cdot X_A}{K C_{AO} (1-X_A)} = \frac{F_R}{K C_{AO} (1-X_A)}$$

→  $F_R$  is known from problem statement.

#  $C_T = \frac{F_R C_M}{K C_{AO} (1-X_A)} + \frac{F_R C_R}{X_A}$  → OBJECTIVE FUNCTION.

#  $\frac{\partial C_T}{\partial X_A} = 0$

#  $V_{opt} = \frac{F_{AO} \cdot X_{A,opt}}{K C_{AO} (1-X_{A,opt})}$

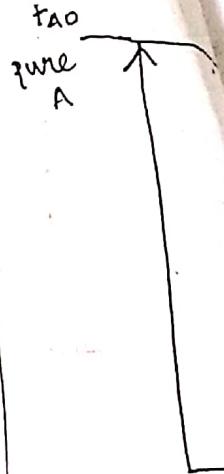
# Calculate the cost of product =  $C_T = \frac{V_{opt} C_M + F_{AO} C_R}{F_R} \cdot F_R$

$$\left( \frac{Rs/hr}{kmol/hr} \right) = \frac{Rs}{kmol}$$

Conversion is usually 70-75%. due to impurities and extra products, thus separators are used.

COST CAN ALSO BE CALCULATED INCLUDING SEPARATION COST.

Separation cost will increase the Product cost.

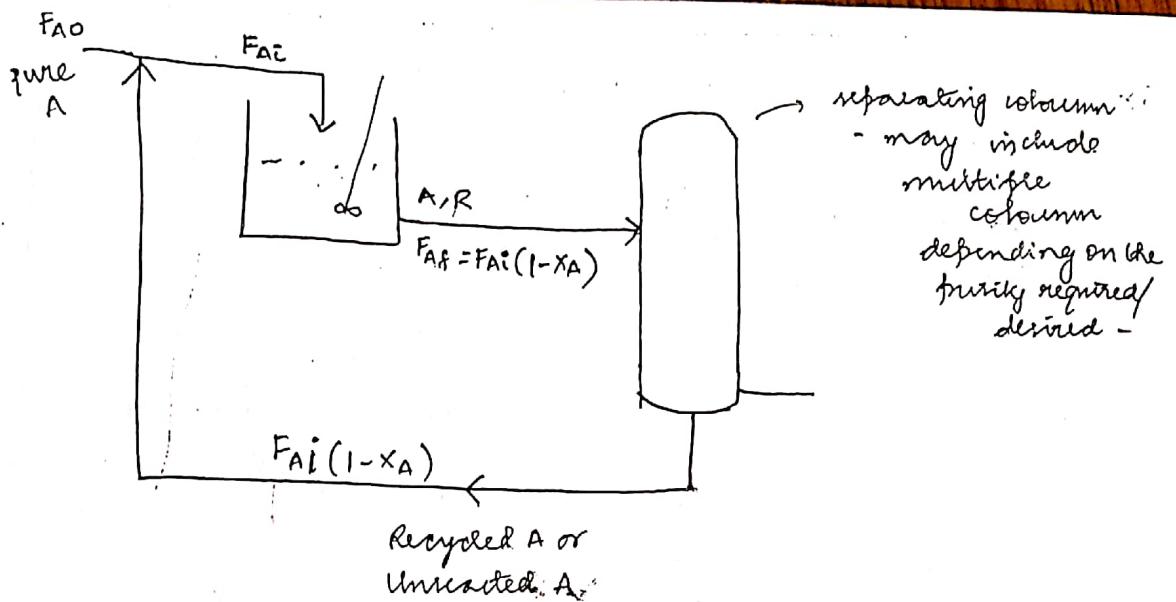


$V_R =$

$F_{AO}$

$F_{AR}$

Ref



$$\therefore C_T = V_R C_M + F_{AO} \cdot C_R + F_{Ai} (1-x_A) C_S$$

$C_S$  = unit cost of separation

$$\therefore V_R = \frac{F_{Ai} \cdot x_A}{K C_{AO} (1-x_A)}$$

$$F_{AO} = F_{Ai} (1-x_A) + F_{AO}$$

$$F_{AO} = \frac{F_{AO}}{x_A}$$

$$\therefore V_R = \frac{F_{AO}}{K C_{AO} (1-x_A)}$$

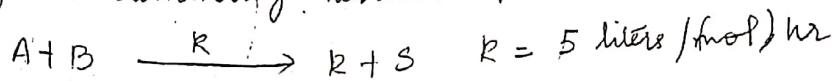
Replacing  $F_{Ai}$  with  $F_{AO}/x_A$  :-

$$C_T = V_R C_M + F_{AO} \cdot C_R + \frac{F_{AO}}{x_A} (1-x_A) C_S$$

$$\frac{dC_T}{dx_A} = 0$$

Find  $x_{A,\text{opt}}$

5) 100 moles of A per hour are available in a concentration of 0.1 mol/lit by a previous process. This stream is to be reacted with B to produce R and S, by the following aqueous phase elementary reaction:

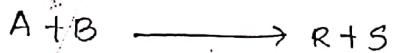


The amount of R required is 95 mol/hr. In extracting R from the reacted mixture A and B are destroyed, hence recycle of unused reactants is out of question. Calculate the optimum reactor size and type as well as feed composition for this process.

Data: B costs ₹ 56.25/mol in crystalline form. It is slightly soluble in the aqueous solution and even when present in large amounts does not change the concentration of A in solution.

Capital and operating costs are ₹ 0.68 hr/liter for PFR and ₹ 0.18/hr.lit for mixed flow reactors.

Soln: Basis: 1 hr operation of CSTR



$$-r_A = -r_B = K C_A C_B = 5 C_A C_B$$

$$\text{As } C_{A_0} X_A = C_{B_0} X_B$$

$$-r_A = 5 C_{A_0}^2 (1-X_A)(M-X_A)$$

$$M = \frac{C_{B_0}}{C_{A_0}} = \frac{C_{B_0}}{0.1} = 10 C_{B_0}$$

$$\frac{V}{v_0} = \frac{C_{A_0} X_A}{-r_A} = \frac{C_{B_0} X_B}{-r_B}$$

$$F_{B_0} = \frac{-r_B V}{X_B} = \frac{5 C_{A_0}^2 (1-X_A)(M-X_A) V C_{B_0}}{C_{A_0} X_A}$$

$$\Rightarrow F_{B_0} \text{ or } C_T = 5$$

$$F_{A_0} X_A =$$

$$F_{B_0} = 1$$

$$V = \frac{10}{K}$$

$$V = \frac{1}{1}$$

$$\therefore C_T =$$

$$10 C_{B_0}$$

$$C_{B_0}$$

$$\Rightarrow F_{BO} = \frac{0.1 C_{AO} - D_0 (1-x_A) (M-x_A)}{x_A}$$

$$C_T = 56.25 \times \left( \frac{5 C_{AO} C_{BO} (1-x_A) (M-x_A)}{x_A} \right) V + 0.18 V$$

assuming R

hence  
calculate  
as feed

P<sub>g</sub>

then  
concentration

for PFR

$$F_{AO} x_A = F_{BO} x_B \Rightarrow x_B = \frac{C_{AO} \cdot x_A}{C_{BO}}$$

$$F_{BO} = \frac{F_{AO} x_A}{C_{AO} \cdot x_A} \cdot C_{BO} = \frac{100}{0.1} C_{BO} = 1000 C_{BO}$$

$$V = \frac{100 x_A}{K C_{AO}^2 (1-x_A) (M-x_A)} = \frac{100 \times 0.95}{5 \times (0.1)^2 (1-0.95) (10 C_{BO} - 0.95)}$$

$$V = \frac{38000}{10 C_{BO} - 0.95}$$

$$\therefore C_T = \frac{56.25 \times 5 \times 0.1 \times C_{BO} (1-0.95) (10 C_{BO} - x_A) \times 38000}{0.95 \times (10 C_{BO} - 0.95)}$$

$$+ 0.18 \times \frac{38000}{10 C_{BO} - 0.95}$$

$$\therefore C_T = 56250 C_{BO} + \frac{6840}{10 C_{BO} - 0.95}$$

$$\frac{\partial C_T}{\partial C_{BO}} = 56250 - \frac{6840 \times 10}{(10 C_{BO} - 0.95)^2} = 0$$

$$10 C_{BO} - 0.95 = \sqrt{\frac{68400}{56250}} = \sqrt{1.28} = 1.103$$

$$C_{BO} = 0.205 \text{ mol / lit}$$

$$C_T = (5625.0 \times 0.205) + \frac{6840}{10 \times 0.205 - 0.95}$$

$$= 11415 + \frac{6840}{1.15} \quad 11531.25 + 6218.2$$

$$= 17749.432$$

$$V = \frac{38000}{10 \times 0.205 - 0.95} = 34545.45 \text{ lit.}$$

For PFR:

$$C_T = 56.25 F_{B_0} + 0.68 V$$

$$V = F_{A_0} \int_0^{0.95} \frac{dx_A}{0.5(1-x_A)(M-x_A)}$$

$$= \frac{2000}{M-1} \left[ -\ln(1-x_A) + \ln(M-x_A) \right]_0^{0.95}$$

$$= \frac{2000}{M-1} \ln \frac{M-0.95}{0.05M}$$

$$\therefore C_T = 56.25 M \times 100 + 0.68 \times \frac{2000}{M-1} \ln \frac{M-0.95}{0.05M}$$

$$F_{B_0} = F_{A_0} \cdot \frac{C_{B_0}}{C_{A_0}} = 100 \cdot M$$

$$\Rightarrow \frac{dC_T}{dM} = 56.25 + \frac{1360}{(M-1)^2} \left[ \frac{0.05M}{M-0.95} \frac{(M-1)}{M^2} \ln \frac{M-0.95}{0.05M} \right] = 0$$

$$\Rightarrow (M-1)^2 \times 56.25 + \frac{1360 \times 0.15 (M-1)}{M(M-0.95)} = 1360 \ln \frac{M-0.95}{0.05M}$$

By trial and error:

$$M = 1.615$$

$$C_{B_0} = 0.161 \text{ mol}$$

$$C_T = 56.25 \times$$

putting the value of  $v_0$ .

$$C_T = 13746.85 \text{ } \frac{\text{M}}{\text{L}}$$

$$V = \frac{2000}{0.615} \ln \frac{1.615 - 0.95}{(0.05)(1.615)}$$

$$= \underline{6856.56 \text{ L}} \quad (\text{PFR when required})$$

- (10) Using a color indicator which shows when the concentration of A falls below 0.1 mol/liter, the following scheme is devised to explore the kinetics of the decomposition of A. A feed of 0.6 mol A liter is introduced into the 1<sup>st</sup> reactor of the 2 mixed reactors in series, each having a volume of 400 cm<sup>3</sup>. The color change occurs in the first reactor for a steady state feed rate of 10 cm<sup>3</sup>/min, and in the second reactor for a steady state feed rate of 50 cm<sup>3</sup>/min. Find the rate (of reaction) equation for the decomposition of A from this information.

Solution:

$$C_{AO} = 0.6 \text{ moles/liter}$$

$$V = 400 \text{ cm}^3 = 0.4 \text{ liter}$$

# (mole balance  
for 2 reactors)

# assume  $F_A = K C_A^n$   
empirical rate  
equation

From reactor ①

$$\frac{V}{F_{AO}} = \frac{V}{V_0 C_{AO}} = \frac{X_A}{K C_A^n} = \frac{C_{AO} - C_A}{C_{AO} \cdot K C_A^n}$$

$$\Rightarrow \frac{V}{V_0} = \frac{C_{AO} - C_A}{K C_A^n}$$

$$\Rightarrow \frac{0.4}{0.01} \frac{\text{liter}}{\text{lit/min}} = \frac{0.6 - 0.1}{K (0.1)^n}$$

$$\boxed{K (0.1)^n = \frac{0.5}{0.4} \times 0.1 = 0.0125} \quad \text{--- 1}$$

For second reaction

$$\frac{V}{V_0} = \frac{C_{A1} - C_{A2}}{KC_{A2}^n} = \frac{0.4}{0.05} = 8 \quad \textcircled{2} \quad \frac{C_{A2}}{C_{A0}} = \frac{0.6}{0.1}$$

$$\frac{V}{V_0} = 8 = \frac{C_{A0} - C_{A1}}{KC_{A1}^n} \quad \textcircled{3}$$

$$\frac{C_{A1} - 0.1}{KC(0.1)^n} = 8$$

$$\textcircled{2} \rightarrow C_{A1} = (8 \times 0.125) + 0.1 = 0.2$$

$$\textcircled{3} \rightarrow C_{A0} - C_{A1} = 8 \times K(C_{A1})^n - KC_{A1}^n$$

$$C_{A0} - 0.2 = 8 K(0.2)^n$$

$$\textcircled{1} \quad \textcircled{5} \quad \frac{K(0.1)^n}{K(0.2)^n} = 0.25$$

$$n \log 0.5 = \log 0.25$$

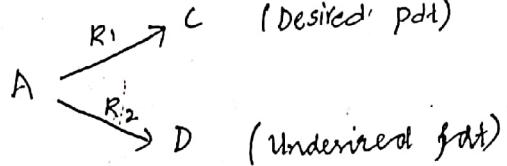
$$n = 2$$

$$K = 1.25$$

$$-\dot{V}_A = 1.25 C_A^2$$

# Multiple Reactions

## - DESIGN OF PARALLEL REACTION -

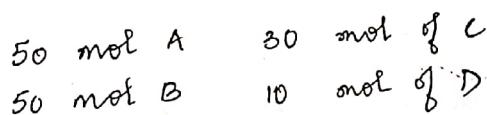
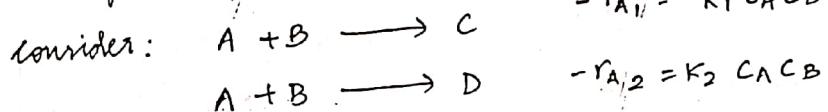


For multiple reactions we need to see three factors :

- (1) CONVERSION
- (2) SELECTIVITY
- (3) YIELD

For single reactions we plot conversion, but for multiple reactions we need to plot selectivity and yield too.

- SELECTIVITY : It is always based on desired product if the selectivity of catalyst is constant, if it is a good catalyst.



$$\text{conversion} = \frac{\text{total moles A converted}}{\text{total moles A supplied}}$$

$$\text{Selectivity of } C = \frac{\text{Total moles of } C \text{ formed}}{\text{Total moles of } D \text{ formed}} \quad (\text{selectivity of } C \\ \text{w.r.t. D - })$$

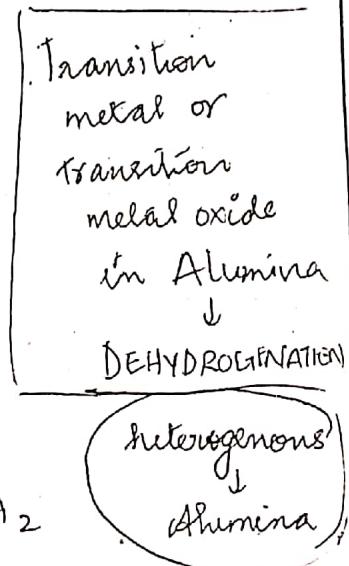
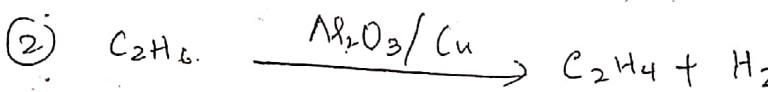
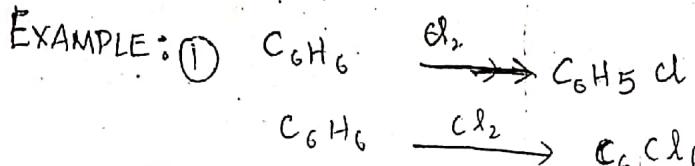
Why is selectivity used w.r.t. some product?  
 If there are multiple reactions we will need to mention selectivity w.r.t. which product.

Under multiple reactions we have parallel and series.  
 1st we will do the design of reactors in case of parallel reactions and we will 1st do the qualitative analysis.

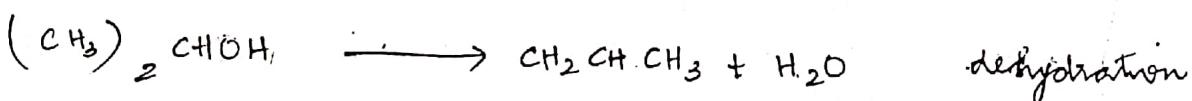
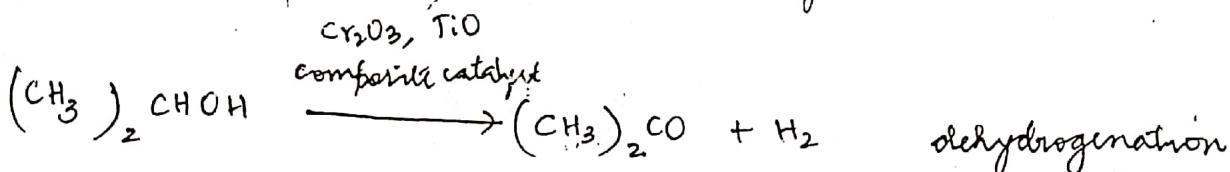
$$\text{Yield of C} = \frac{\text{moles of C formed}}{\text{moles of A reacted (supplied)}} \times 100$$

but not converted

$$= \frac{30}{60} \times 100 = 60\%$$



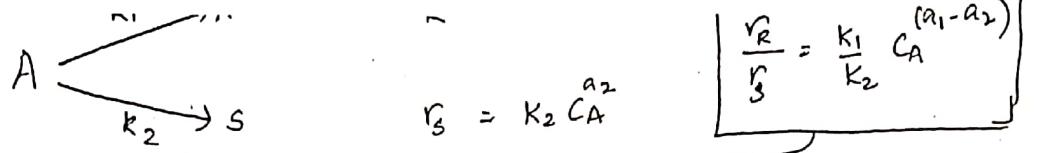
oxyacetylene flame;  $\text{C}_2\text{H}_4$  is one derived product should be designed in such a way that rate constant for 2nd reaction decreases.



Dehydrogenation of Isopropanol  $\rightarrow$  acetone is produced

Deactivating product  $\rightarrow$  adsorbs on active sites, conversion decreases  $\rightarrow$  Disadvantage of parallel reactions.

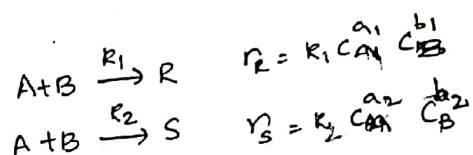
not  
invited



- CASE 1 : IF  $(a_1 - a_2) > 0$  (+ve) with ↑ in concentration  
                   ↑ selectivity of 'R' ↑
- CASE 2 : If  $(a_1 - a_2) < 0$  (-ve) " " "
- CASE 3 :  $(a_1 - a_2) = 0$  " " independent of concentration

If 2 reactants are involved :

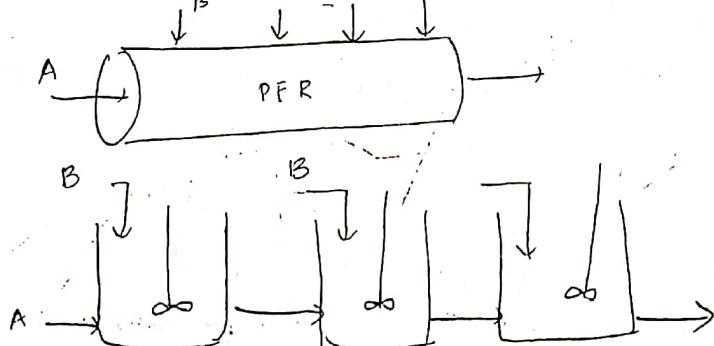
$$\frac{r_R}{r_S} = \frac{k_1}{k_2} C_A^{(a_1-a_2)} C_B^{(b_1-b_2)}$$



case (1) : A, B with high  
                   Batch reactor : A, B added at same time

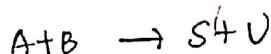
case (2) : A, B both low

case (3) : A is high      B is low



### Reacting scheme

example : select desirable scheme



B to be kept long  
                   A → main stream

$$\frac{r_S}{r_R} = \frac{k_2}{k_1} C_A^{-0.5} C_B^{1.5}$$

## EXOTHERMIC REACTIONS

Instantaneous yield :

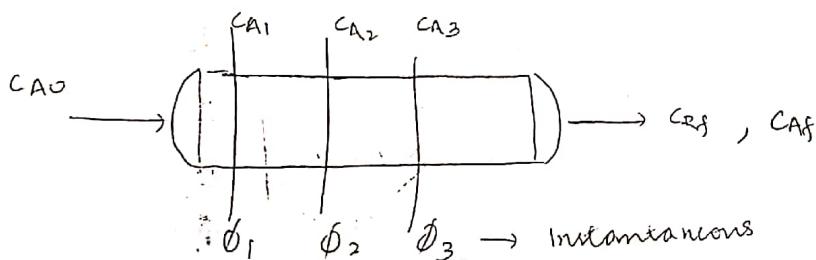
$$\phi = \frac{\text{moles of R formed}}{\text{moles of A reacted}} = \frac{dC_R}{-dC_A} = \text{instantaneous yield of R}$$

$\phi$  will vary along the length of PFR as  $x$  increases

Overall yield :

$$\Phi = \frac{\text{all R formed}}{\text{all A reacted}} = \frac{C_{RF}}{C_{AO} - C_{AF}} = \frac{C_{RF}}{-\Delta C_A}$$

Exit concentration of R is  $C_{RF}$



In mixed reaction,  $C_{RF} = \Phi (C_{AO} - C_{AF})$

and in PFR,  $\Phi = \frac{dC_R}{-dC_A}$

$$C_{RF} = - \int_{CA_0}^{CA_S} \Phi dC_A$$

$\Phi$  is a function of concentration, as concentration varies,  $\Phi$  will change.

$$\Phi = f(C_A)$$

Example:



$$\Phi \uparrow$$

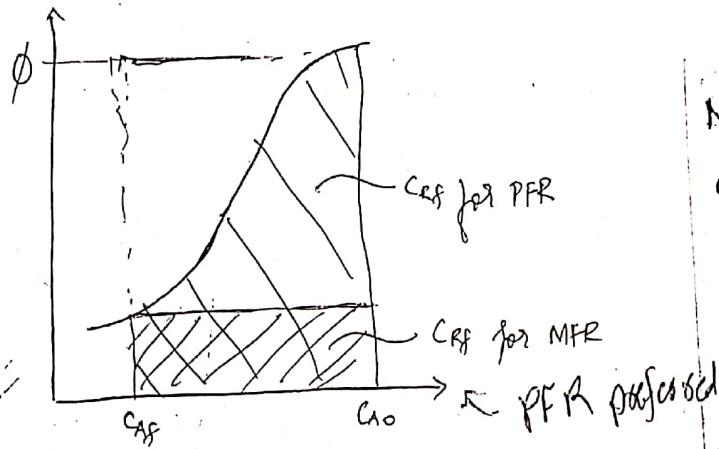


In mixed reactor  $C_{RF} = \phi(C_{A0} - C_A)$

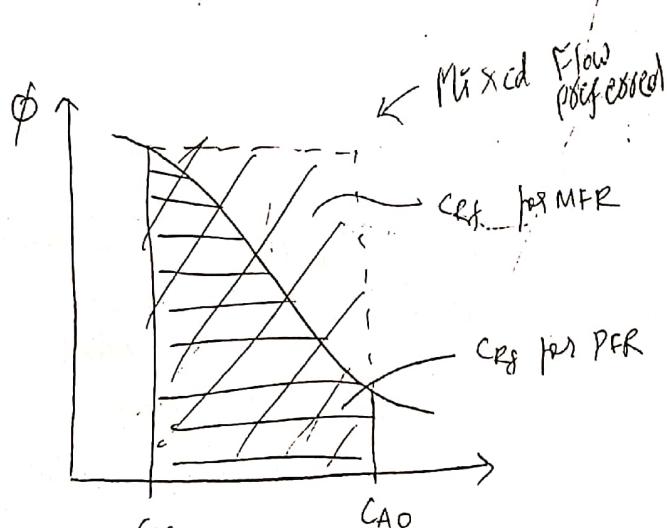
In PFR  $C_{RF} = - \int_{C_{A0}}^{C_A} \phi dC_A$

$$\phi = f(C_A)$$

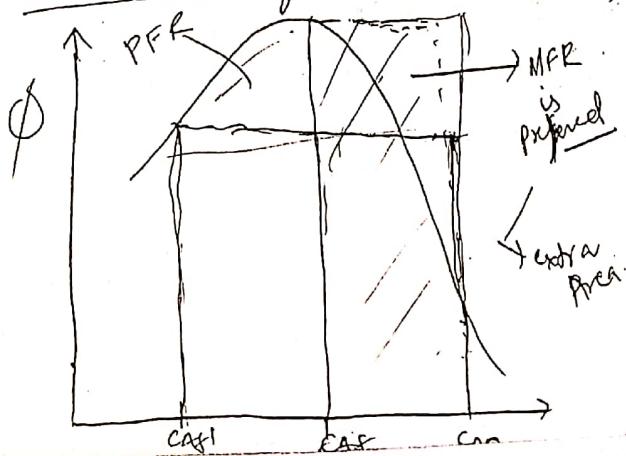
Example:  $\phi = \frac{1}{1+2C_A^2}$  or  $\phi = \frac{C_A^2}{C_A + 3C_A^2}$



NATURE OF THE CURVE WILL DECIDE WHICH REACTOR WILL HAVE LOWER OR HIGHER  $C_{RF}$



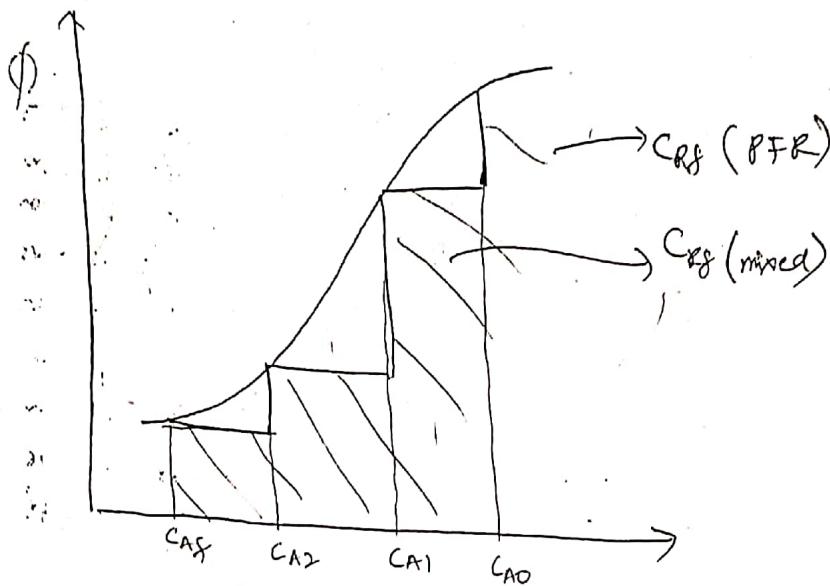
Autocatalytic reactions  $\rightarrow$



We have to optimise

Solve

Equations relating to only the two equations



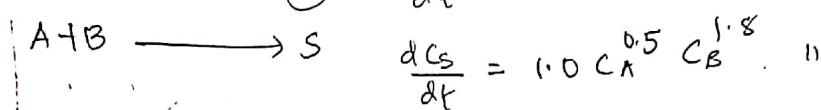
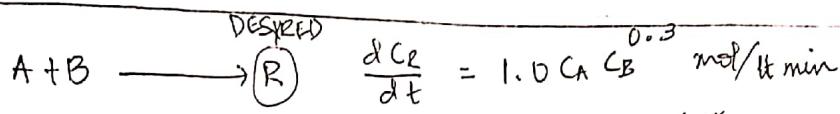
$$\Phi_p =$$

$\Phi_p$  is used to

AB C

$$\Phi_p$$

### PROBLEM



Find the fraction of impurities in the product stream  
from 90% conversion of pure A and B (each stream has a conc of  
20 mol/lit):

(a) for PFR      (b) for MFR

(c) for plug flow-mixed combination if  $C_B$  is added such  
that it is diluted to 1 mol/lit.

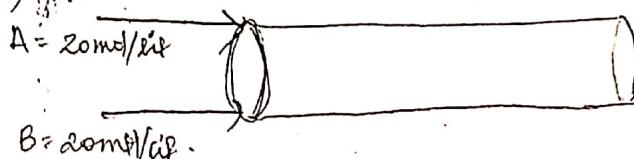
Solution:

① Write instantaneous yield:

$$\phi = \frac{dC_R}{dC_{Rf} dC_S} = \frac{R_1 C_A C_B^{0.3}}{R_1 C_A C_B^{0.3} + R_2 C_A^{0.5} C_B^{1.8}}$$

$$= \frac{1}{1 + C_A^{-0.5} C_B^{1.5}}$$

(a) FOR PFR



Fraction

Concentration

$$C_{Rf}$$

$$C_{Rg}$$

$$\Phi_p = \frac{C_{RF}}{C_{AO} - C_{AF}} = -\frac{1}{C_{AO} - C_{AF}} \int_{C_{AO}}^{C_{AF}} \phi dC_A$$

$$= -\frac{1}{10-1} \int_0^1 \frac{1}{1 + \bar{C}_{AO}^{0.5} C_B^{1.5}} dC_A$$

$\Phi_p$  is used to calculate the fractional impurities.

As  $C_A = C_B$  everywhere :-

$$\begin{aligned}\bar{\Phi}_p &= -\frac{1}{10-1} \int_0^1 \frac{1}{1 + \bar{C}_A^{0.5} C_A^{1.5}} dC_A \\ &= \frac{1}{9} \int_0^1 \frac{dC_A}{1 + C_A} \\ &= \frac{1}{9} \ln(1 + C_A) \Big|_0^1 \\ \bar{\Phi}_p &= 0.19\end{aligned}$$

$$\text{Fraction of impurities} = 1 - \bar{\Phi}_p = 0.81 = \underline{\underline{81\%}}$$

Concentration of Products :-

$$C_{RF} = (C_{AO} - C_{AF}) \bar{\Phi}_p$$

$$= (10-1) 0.19$$

$$= 1.71 \text{ mol/lit}$$

$$C_{RF} = (C_{AO} - C_{AF})(1 - \bar{\Phi}_p)$$

$$= (10-1) 0.81$$

$$= 7.29 \text{ mol/lit}$$

$$\phi|_{C_{AS}} = \frac{1}{1+C_{Af}} = \frac{1}{1+1} = \frac{1}{1+1} = 0.5$$

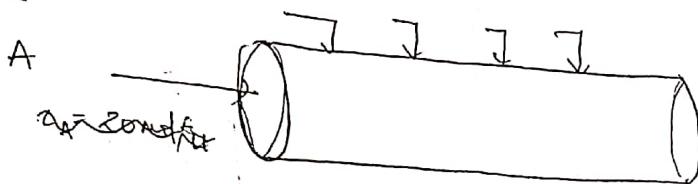
Inflow rate = 50%.

For MFR we evaluate  $\phi$  at exit:

$$\phi = \frac{1}{C_{Af} + 1 + C_A} \approx \frac{1}{1 + C_{Af}}$$

~~Enter~~ ~~Exit~~

(c)



$$C_{B0} = 1 \text{ mol/lit.} \quad C_{Af} = 1 \\ C_{AO} = 19 \text{ mol/lit.}$$

$$\phi = -\frac{1}{C_{AO} - C_{Af}} \int_{19}^1 \frac{dC_A}{1 + C_A^{-0.5}} C_B^{1.5} \quad C_B = 1$$

$$= \frac{4}{18} \int_1^{19} \frac{dC_A}{1 + C_A^{-0.5}} = \frac{1}{18} \left[ (19-1) - 2(\sqrt{19} - 1) + 2 \ln \frac{1+\sqrt{19}}{2} \right] \\ = 0.74$$

Questions — maximum yield  $\rightarrow$  Find Optimum  $\phi$   
 A  $\xrightarrow{R} R_1 C_A = r_e$   
 A  $\xrightarrow{S} R_2 C_A = r_s \rightarrow$  Desired product fraction desired  $\phi$ .  
 A  $\xrightarrow{T} R_3 C_A = r_T$

$$\phi_{opt}(C_A) = \frac{r_s}{r_e + r_s + r_T} = f(C_A)$$

$$\left( \frac{d\phi}{dC_A} = f'(C_A) = 0 \right) \quad \phi_{opt} = 2$$

$$C_{sf\max} = ?$$

write expression for  $C_s$

$$\frac{dC_{sf}}{dC_A} \rightarrow C_{s\max}$$

For MFR

$$\textcircled{1} \quad C_{sf} = \phi\left(\frac{s}{A}\right)(-\Delta C_A)$$

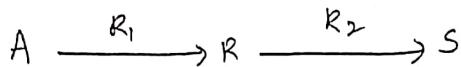
$$\textcircled{2} \quad \frac{dC_{sf}}{dC_A} = \dots \quad (\text{big exp})$$

We will remove  $C_A$  off from this expression.

we will get  $C_{sf\max}$ .

# SEKIES MULTIPLEX REACTIVITY

(Qualitative Analysis)



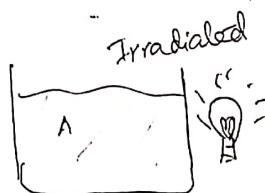
$$-r_A = R_1 C_A$$

$$+r_R = k_1 C_A - k_2 C_R$$

$$r_S = R_2 C_R$$

Series reaction  
1st order  
 $R_1, R_2$  rate constants ( $\text{L mol}^{-1} \text{s}^{-1}$ )

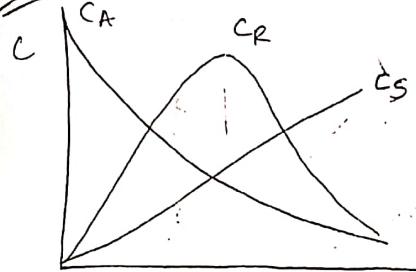
SUPPOSE IT IS A LIGHT SENSITIVE REACTION (light on reaction vessel)  
light off " stops



As R forms, A & R will fight for light

~~It's similar to Batch reactor & PFR.~~

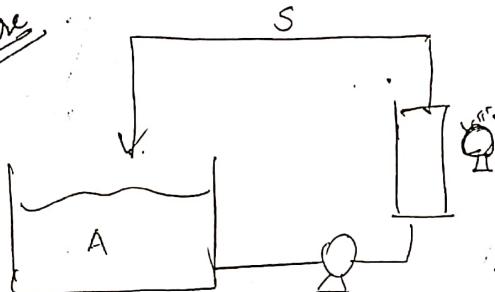
1st CASE



irradiation carried out in system  $\rightarrow$  R is maximum,  
entire stream is reacted.

Behavior of Batch & PFR  
 $\rightarrow$  R is Desired product.

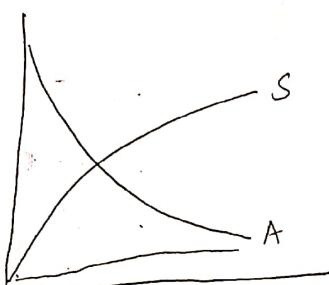
2nd case



Our product will be 'S'

R will be in traces.

'S' AS DESIRED PRODUCT



(THEORY + PROB Imp in this chapter)

Amount of mixing  $\propto$  (Formation of Intermediate) $^{-1}$   
Batch/Plug Flow  $\leftrightarrow$  Intermediate (desired) R  
CSTR  $\leftrightarrow$  Final (desired) S

Vant Gogh  
Series

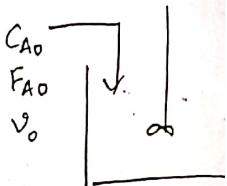
a) PFR

$$\frac{C_{R,\max}}{C_{A,0}} = \left( \frac{k_1}{k_2} \right)$$

$$C_{\text{prop}} = \frac{1}{K_{\text{hydro}}}$$

$$C_{\text{prop}} = \ln \left( \frac{1}{k_2} \right)$$

b) MFR



$$\frac{dC_R}{dZ_m} = 0$$

$$Z_{m,\text{opt}} = \frac{1}{\sqrt{K}}$$

$$\frac{C_{R,\max}}{C_{A,0}} = \frac{1}{1}$$

A balance

$$\frac{C_A}{C_{A,0}} = v C$$

$$\frac{C_A}{C_{A,0}} = \frac{1}{1}$$

## Variative Analysis

### Series



$$\frac{C_{R,\max}}{C_{A_0}} = \left(\frac{k_1}{k_2}\right)^{\frac{k_2}{k_2-k_1}}$$

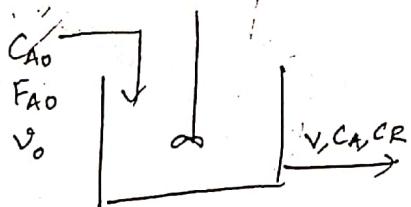
$$\frac{C_A}{C_{A_0}} = e^{-k_1 z}$$

$$\frac{C_R}{C_{A_0}} = \frac{k_1}{k_2 - k_1} (e^{-k_1 z} - e^{-k_2 z})$$

$$z_{\text{bott}} = \frac{1}{K_2 \text{mean}}$$

$$z_{\text{poff}} = \frac{\ln(k_2/k_1)}{k_2 - k_1} \quad (1)$$

### b) MFR



$$C_S = C_{A_0} - C_A - C_R$$

$$\frac{C_R}{C_{A_0}} = \frac{k_1 k_2 z_m^2}{(1 + k_1 z_m)(1 + k_2 z_m)}$$

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

$$\frac{dC_R}{dz_m} = 0$$

$$z_{m,\text{opt}} = \frac{1}{\sqrt{k_1 k_2}} \quad (2)$$

$$\frac{C_{R,\max}}{C_{A_0}} = \frac{1}{\left[\left(\frac{k_2}{k_1}\right)^{\frac{k_2}{k_2-k_1}} + 1\right]^2} \quad (3)$$

### R-balance

$$\nabla C_{R0} = \nabla C_E + (-r_E) \nabla$$

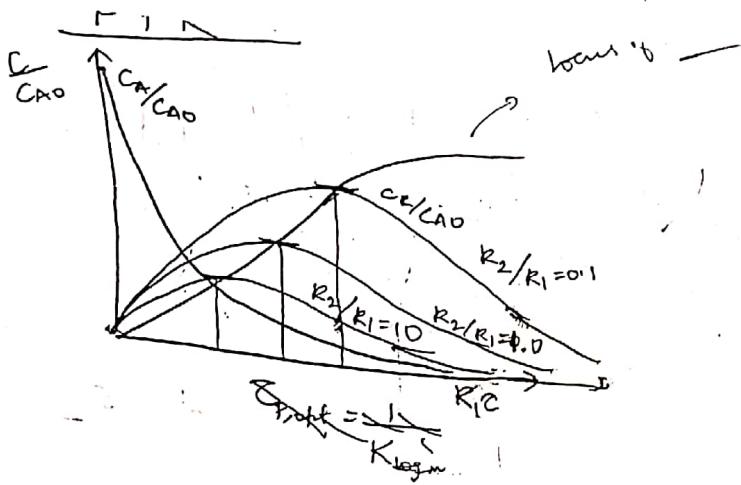
$$0 = \nabla C_E + (-k_1 C_A + k_2 C_R) \nabla$$

$$C_R \left( k_2 + \frac{1}{z_m} \right) = \frac{k_1 C_{A_0}}{1 + k_1 z_m}$$

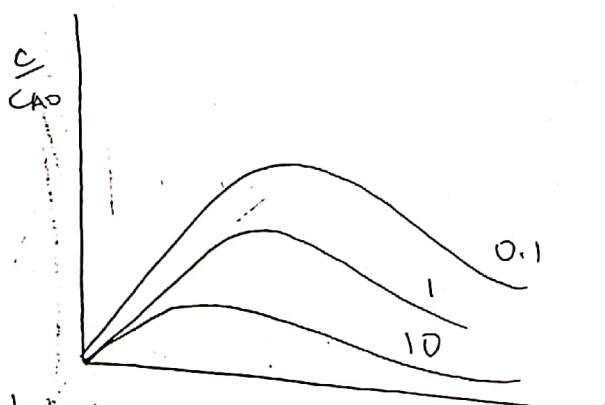
### A-balance

$$\nabla C_{A0} = \nabla C_A + k_1 C_A V$$

$$\frac{C_A}{C_{A_0}} = \frac{1}{1 + k_1 z_m}$$



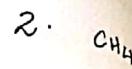
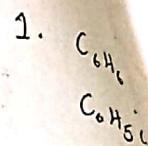
MFR



17/10/19

instantaneous yield vs conversion

of the plots for CSTR & PFR are plotted together MFR will always be lower than PFR So if our desired product is R' then PFR is PREFERRED!



General

1.  $A + B \xrightarrow{k_1/k_2}$  Product
2.  $R + B \xrightarrow{k}$  Product

Qualitative cases

- ① A slowly add solution of
- ② B slowly add solution of
- ③ A and B

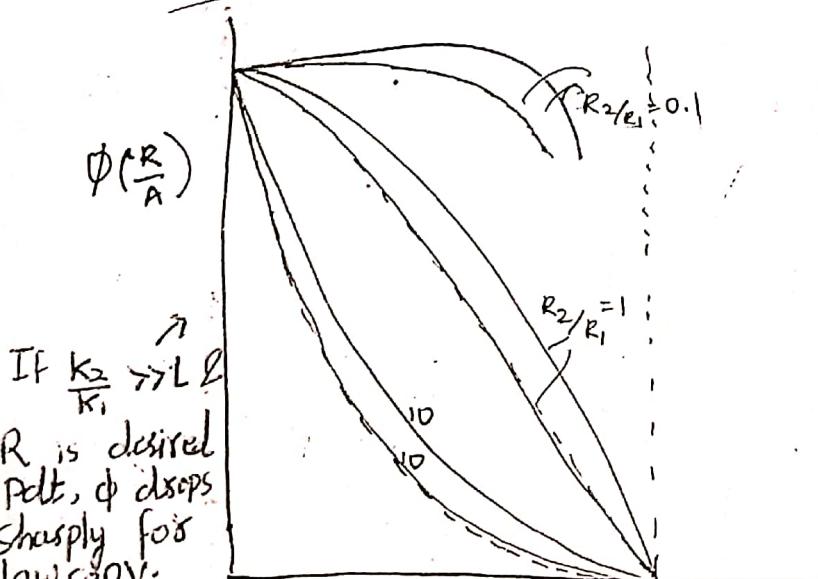
Case A

$\rightarrow$  B is

PFR  
MFR

If  $k_2/k_1$  is large low conversion levels are chosen to get high  $\phi$

$\downarrow$   
conversion is low  
 $\therefore$  large reactor required



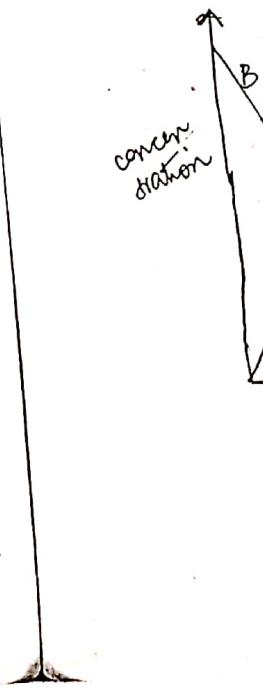
If  $k_2/k_1 \gg 1$   
R is desired Pdt,  $\phi$  drops sharply for low conv.

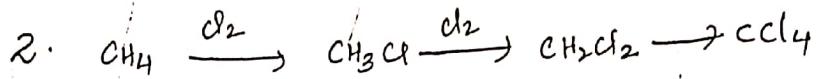
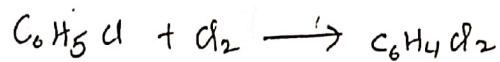
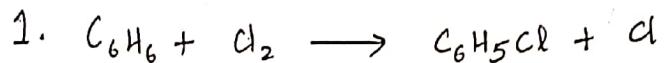
For avoiding escalation of S, we design for low conversion  $X_A = 1 - \frac{C_A}{C_A + 2}$

so, large theoretical quantities related to Design - when we will chose which how?

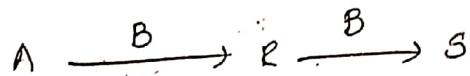
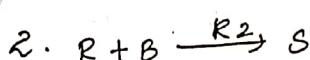
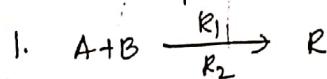
qnty of materials  $\rightarrow$  here large reactors will be there & cost ↑

If  $k_2/k_1 < 1$ , we focus on high conversion of A





General form



$$\frac{dC_A}{dt} = -\text{R}_1 \text{C}_A \text{C}_B$$

$$\frac{dC_B}{dt} = -\text{R}_1 \text{C}_A \text{C}_B - \text{R}_2 \text{C}_R \text{C}_B$$

$$\frac{dC_S}{dt} = \text{R}_2 \text{C}_R \text{C}_B = \frac{dC_S}{dt}$$

$$\text{R}_R = \text{R}_1 \text{C}_A \text{C}_B - \text{R}_2 \text{C}_R \text{C}_B$$

Qualitative cases :-

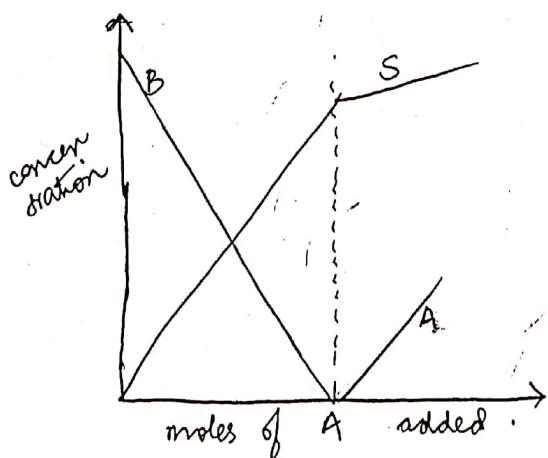
(1) A slowly added to a solution of B

(2) B slowly added to a solution of A

(3) A and B both rapidly mixed together

Case A A slowly added to a solution of B.

→ B is largely available

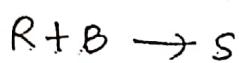


(no R → because small amount of A is added to excess B)

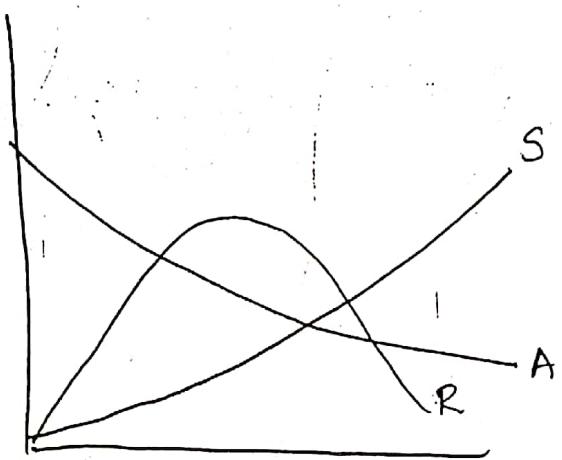
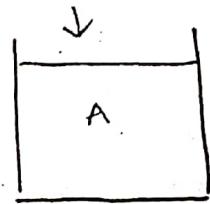
B is in large amount so all of R formed will react with B no competition b/w A & R because B is excess.

When we add  
choose which  
how?

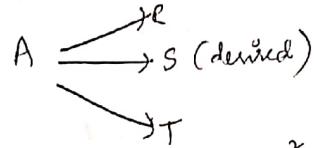
(b) Drawing when  $\alpha$  is varying



A and R will compete for B.



Q. If reactant A decomposes as per the following reaction



with  $r_E = 1$ ,  $r_S = 2CA$ ,  $r_T = CA^2$ , Take  $C_{AO} = 2 \text{ mol/l}$

Determine the minimum concentration of desired product ( $C_S$ ) that can be obtained

- (i) In a mixed flow reactor
- (ii) in a plug flow reactor

1<sup>st</sup> → find instantaneous yield

$$\Phi\left(\frac{S}{A}\right) = \frac{r_S}{r_S + r_E + r_T} = \frac{dC_S}{dC_S + dC_A + dC_T} = \frac{2CA}{1+2CA+CA^2}$$

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

$$\frac{d\Phi}{dC_A} = \frac{2}{dC_A} \left( \frac{CA}{(1+CA)^2} \right) = 0$$

What is the maximum fractional yield?

$$1 + CA - 2CA = 0$$

$$CA = 1.0 \quad \boxed{CA = 1} \quad \text{for maximum } \Phi$$

$$\Phi_{max} = \frac{2}{1+2+1} = 0.5$$

MIXED REACTOR for  $C_{AO} = 2$

$$C_{sf} = \Phi\left(\frac{S}{A}\right)(-dC_A) = \frac{2CA}{(1+CA)^2} (C_{AO} - CA)$$

$$= 4CA - 2CA^2$$

$$\frac{dC_{sf}}{dC_A} = 2 \frac{d}{dC_A} \left( \frac{2CA - CA^2}{(1+CA)^2} \right) = 0$$

$$4 \left[ \frac{(1-CA)(1+CA) - (2CA - CA^2)}{(1+CA)^3} \right] \quad C_{AO} = 2$$

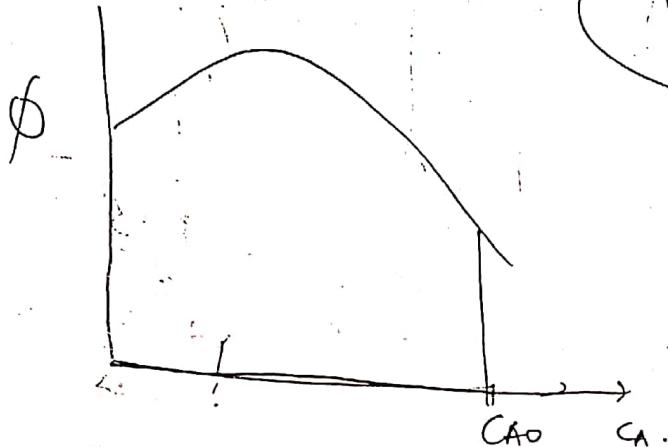
$$1 - CA^2 + 2CA - CA^2 = 0 \quad CA_{opt} = 0.5$$

$$C_{sf, \max} = \frac{2 C_A}{(1+C_A)^2} (C_{A0} - C_A) \Big|_{C_A=0.5} = 0.666$$

21/10/15

- Local Behavior
- (1) No
  - (2) Complete
- Behavior
- 

PFR



We have to see  
when we get  
maximum

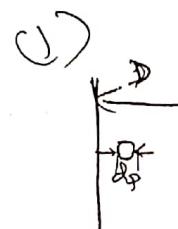
when  
 $C_A = 0$ .

→ Monotonic  
Deviation

(1) Element  
conservation

(2) Create  
aggregates

(3) Use  
of PFR



$$C_{sf} = - \int_{0}^{1} \Phi dC_A$$

$$= \int_0^2 \frac{2 C_A}{(1+C_A)^2} dC_A$$

$$= 2 \left[ \ln x + 2 \int_0^2 \frac{(x-1)}{x^2} dx \right]$$

$$= 2 \left\{ \ln x - \frac{1}{2} \right\}$$

$$= 0.864$$

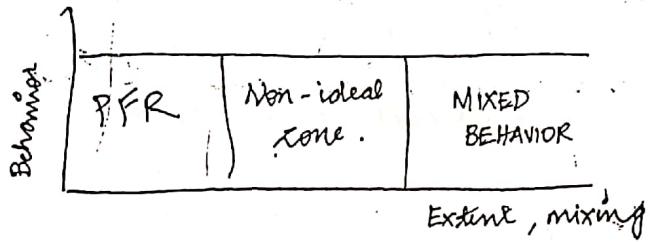
Seg

# 0/10/15 - NON-IDEAL REACTORS -

*Behaviors*  
axial  
we get  
minimum  
when  
 $C_A = 0$ .

Ideal Behavior:

- (1) No axial mixing (PFR)
- (2) Complete mixing (ideal CSTR)



What are causes of Non-Ideal Behavior?

Derivation from ideal behavior are due to following reasons:

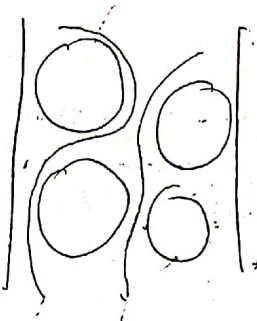
- (1) Element of fluid may move at different velocities causing channeling.
- (2) Creation of stagnant point or dead spots or partially aggregated segregated as they move.
- (3) The extent of micromixing, diffusion in the direction of flow or dispersion.

(1)

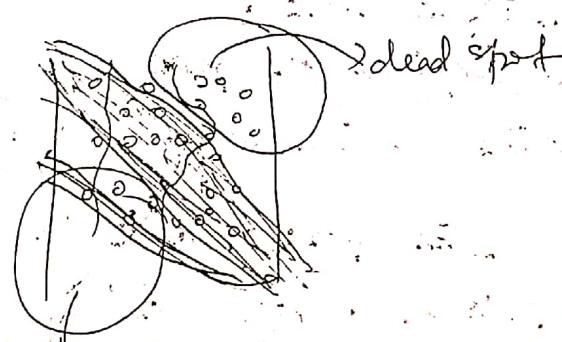


$$\frac{dp}{D} = \frac{1}{10}$$

particles should be within this range or channeling will occur.

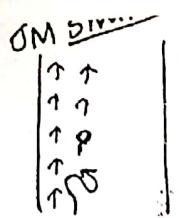


Segregated - laminar profile



dead spot

volume is not utilized by the reactants.



Dispersion (dispersion coefficient)  $\frac{De}{UL}$  (similar to  $P_e$ )  
 micromixing dispersion number  $\frac{De}{UL}$

\* There can be large numbers of different mixing state depending on micromixing and segregation.

\* Four methods are used to determine these deviations.

### (CELL BALANCE METHOD).

1. Segregated flow model
2. Dispersion model
3. CSTR in series model
4. Recycle Reactor model

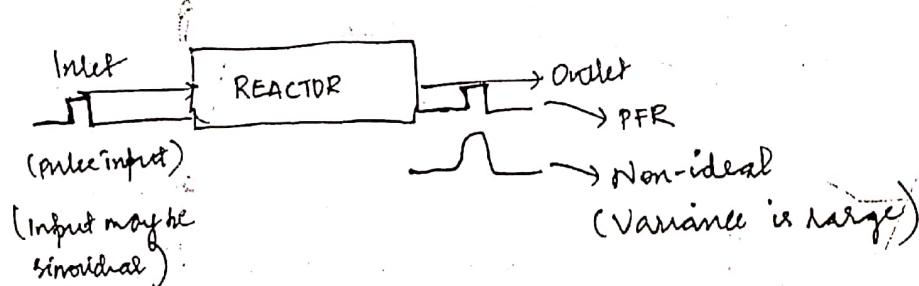
theoretical model.

$$T = \Delta t$$

$$\Theta = De$$

### PROBLEM

Substance following



### RESIDENCE TIME :

Time required to process 1 volume

particles coming early - stay longer - more reaction - more conversion

(Examples: Students in class)

Non-ideal - diff Residence times

Ideal - Same residence time.

The feed

$$C_{R0} = C_0$$

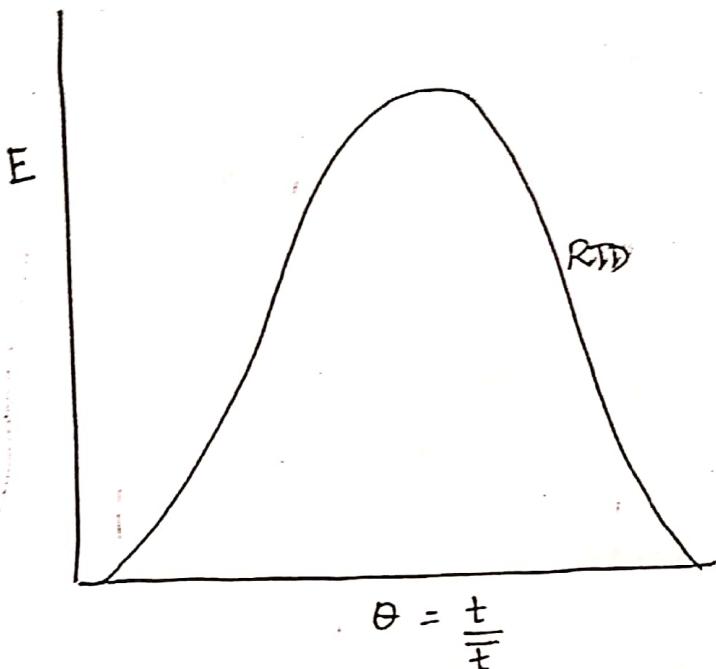
$$C_2 = 10 \text{ m}$$

$$C_{R1} = 0$$

$$C_{S1} = 0$$

Find the

$$\frac{C_{R0}}{C_{R0} - C_{S0}} = \frac{C_1}{C_2}$$

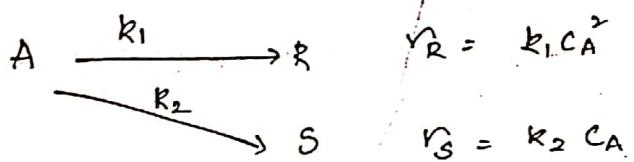


$\bar{t}$  = Average residence time

$\theta$  = Dimensionless time

### PROBLEM

Substance A in the liquid phase produces R and S by the following reactions:



The feed containing  $C_{A0} = 1.0 \text{ mol/l}$

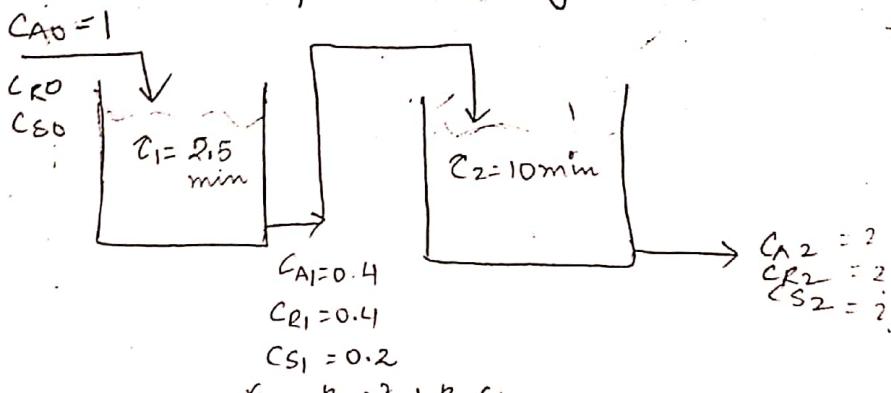
$C_{R0} = C_{S0} = 0$  enter two CSTR in series ( $\tau_1 = 2.5 \text{ min}$

$\tau_2 = 10 \text{ min}$ ).  $C_{A1} = 0.4 \text{ mole/l}$

$$C_{R1} = 0.4 \text{ moles/l}$$

$$C_{S1} = 0.2 \text{ moles/l}$$

Find the composition leaving second reactor.



CSTR 1

$$\frac{V}{F} = \frac{C_{A0} - C_{A1}}{(-r_A)_1} = \frac{A \text{ balance}}{C_1 = 2.5 = \frac{1 - 0.4}{R_1(0.4)^2 + R_2(0.4)}} \quad \text{--- (1)}$$

From eq 1  
 $10 C_{A2}^2$   
 $C_{A2} =$

R balance

$$\frac{V}{F} = \frac{C_{R1} - C_{R0}}{(r_R)_1} = 2.5 = \frac{0.4}{R_1(0.4)^2} = R_1 = 1$$

S balance

From eq (2)

\* Putting  $R_1$  value in equation (1) :-

$$R_2 = \frac{1 - 0.4}{2.5} - R_1(0.4)^2$$

$$= 0.08 \text{ min}^{-1}$$

$$0.4 R_1 + R_2 = 0.6$$

$$R_2 = 0.6 - 0.4 = 0.2$$

from eq (3)

CSTR 2

A balance

$$\frac{V}{F} = C_2 = \frac{C_{A1} - C_{A2}}{(-r_A)_2} = 10 = \frac{0.4 - C_{A2}}{(1) C_{A2}^2 + (0.08) C_{A2}} \quad \text{--- (1)}$$

A and B

2A

A+B

2B

Find W

R balance

$$C_2 = 10 = \frac{C_{R2} - C_{R1}}{r_R} = \frac{C_{R2} - 0.4}{(1) C_{A2}^2} \quad \text{--- (2)}$$

S balance

$$10 = \frac{C_{S2} - C_{S1}}{r_S} = \frac{C_{S2} - 0.2}{(0.08) C_{A2}} \quad \text{--- (3)}$$

From equation (1) :

$$10C_{A_2}^2 + 3C_{A_2} - 0.4 = 0$$

$$C_{A_2} = \frac{-3 \pm \sqrt{9+16}}{20}$$

$$= 0.1, -0.4 \quad C_{A_2} = 0.1$$

From eq (2) :  $C_{R_2} = 0.5$

$$C_{R_2} = 0.5$$

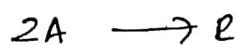
$$C_{L_2} = 0.5$$

$$C_{S_2} = 0.4$$

From eq (3)  $C_{S_2} =$

---

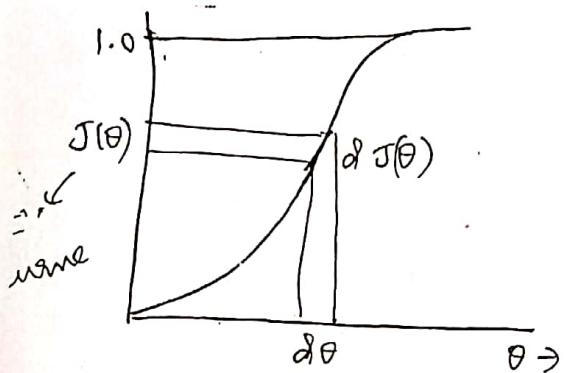
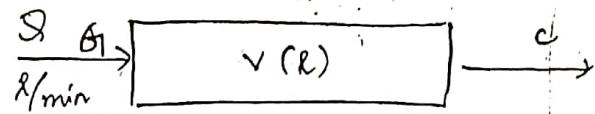
A and B react with each other as follows



Find what ratio of A:B B should be maintained.

34/10/19

$J(\theta)$  fraction of stream have a residence time less than  $\theta$ .  
 $\theta \rightarrow$  residence time.  
At  $\theta = 0$ ,  $J(\theta) = 0$ .



$dJ(\theta)$  is having residence time in between  $\theta$  and  $\theta + d\theta$

$$\bar{\theta} = \frac{\int_0^1 \theta dJ(\theta)}{\int_0^1 dJ(\theta)} = \int_0^1 \theta dJ(\theta) = \frac{V}{Q} \text{ or } \left( \frac{V}{Q} \right) \rightarrow \text{ideal Reactor}$$

$$\frac{dJ(\theta)}{d\theta} = J'(\theta)$$

$$dJ(\theta) = J'(\theta) d\theta$$

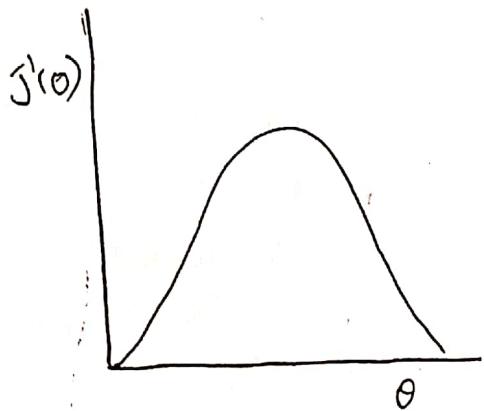
$J'(\theta)$  is called the exit age distribution and designated by 'E'.

E curve is the plot of E vs  $\theta$  or t

*(J.M. Smith)*

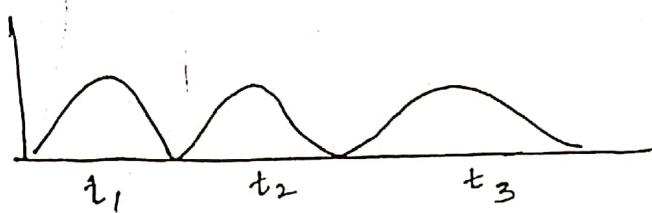
$J'(\theta) \Leftrightarrow E \text{ curve}$

differentiation of 'F' curve  $\rightarrow$  'E' curve.



Distribution curve

Variation of RTD  
Flow behavior  
- Conversion will change



$$\text{Average Residence time } \bar{\theta} = \frac{\int_0^{\infty} \theta J(\theta) d\theta}{\int_0^{\infty} J(\theta) d\theta}$$

$$= \int_0^{\infty} \theta J(\theta) d\theta$$

(Numerical \$ \rightarrow \$

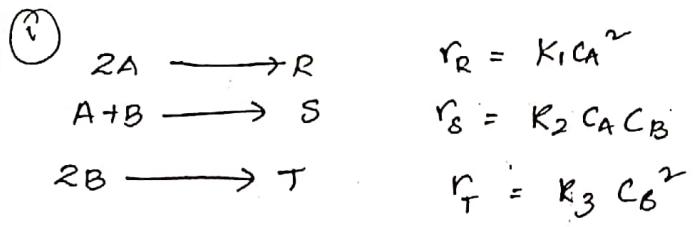
Discrete method

$$\bar{\theta} = \sum \theta E \Delta \theta$$

$$\bar{t} = \sum t E \Delta t$$

t	E	txE	tEDt
0	1	0	0
15	1	15	10
20	1	20	25
25	1	25	30
30	1	30	35
35	1	35	

$\Delta t$  ↓  
Interval  
has to be  
equal



Sis desired  
Product

$$\text{let } \bar{x} = \frac{c_A}{c_B}$$

$$\phi\left(\frac{s}{R+S+T}\right) = \frac{k_2 c_A c_B}{k_1 c_A^2 + k_2 c_A c_B + k_3 c_B^2}$$

$$= \frac{k_2}{k_1 \frac{c_A}{c_B} + k_2 + k_3 \frac{c_B}{c_A}}$$

$$= \frac{k_2 \bar{x}}{k_1 \bar{x}^2 + k_2 \bar{x} + k_3}$$

$$\frac{d\phi}{d\bar{x}} = 0$$

$$(k_1 \bar{x}^2 + k_2 \bar{x} + k_3) k_2 - k_2 \bar{x} (2k_1 \bar{x} + k_2) = 0.$$

$$k_1 k_2 \bar{x}^2 + k_1 k_2 \bar{x} + k_1 k_2 k_3 \bar{x}^2 - 2k_2 k_1 \bar{x}^2 - k_2^2 \bar{x} = 0.$$

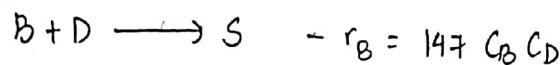
$$k_1 k_2 \bar{x}^2 = k_2 k_3$$

$$\bar{x}^2 = \frac{k_2 k_3}{k_1 k_2} = \frac{k_3}{k_1}$$

$$\therefore \bar{x} = \frac{c_A}{c_B} = \sqrt{\frac{k_3}{k_1}}$$

$$\therefore \text{required ratio of } \frac{c_A}{c_B} \text{ should be } \sqrt{\frac{k_3}{k_1}}$$

Prob 5



Given:

$$\frac{C_{AO}}{C_{BD}} = 9 \quad \frac{C_A}{C_B} = 100 \text{ (at least)}$$

How much D = ?

$$\frac{-\frac{dC_B}{dt}}{-\frac{dC_A}{dt}} = \frac{r_B}{r_A} = \frac{147 C_B C_D}{21 C_A C_D} = \frac{7 C_B}{C_A}$$

$$\Rightarrow \frac{dC_B}{dC_A} = \frac{7 C_B}{C_A}$$

$$\text{or } \int_{C_{B0}}^{C_{Bf}} \frac{1}{7 C_B} dC_B = \int_{C_{A0}}^{C_{Af}} \frac{1}{C_A} dC_A$$

$$\Rightarrow \frac{1}{7} \ln \left( \frac{C_{Bf}}{C_{B0}} \right) = \ln \left( \frac{C_{Af}}{C_{A0}} \right)$$

$$\frac{C_{Af}}{C_{A0}} = \left( \frac{C_{Bf}}{C_{B0}} \right)^{1/7}$$

$$\frac{100 C_{Bf}}{C_{A0}} = \frac{(C_{Bf})^{1/7}}{(C_{B0})^{1/7}}$$

$$C_{Bf}^{1/7} = \frac{C_{A0}}{100} \cdot \frac{1}{C_{B0}^{1/7}} = \frac{45}{100} \times \frac{1}{5^{1/7}}$$

$$C_{Bf}^{1/7} = 0.301$$

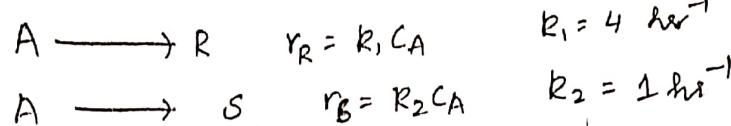
$$C_{Bf} = 0.301 \text{ mol/lit}$$

$$C_{Af} = 30.1 \text{ mol/lit}$$

D consumed per liter = A consumed by 1st reaction + B<sub>1</sub> (2nd reaction)  

$$= (45 - 30.1) + (5 \cdot 0.301) = 19.6 \text{ moles}$$

PROB 0



Given:

$$V = 20 \text{ hr}$$

$$C_{A0} = 1 \text{ mol/l}$$

Profit maximization

Cost of A = 1 \$ per/mol of A

Selling price of R = \$ 1 per mol of R.

S has no value.

Operating cost = 25 \$ per hour

Product separation cost = 1.25 \$ per mol of A fed to reactor

$$\frac{1 - x_A}{x_A} = \frac{k_1}{k_2}$$

$$P = P_{\text{profit}}$$

$$\frac{\partial P}{\partial F_{A0}}$$

Unconverted A is not recycled.

Given: Basis = 1 hour operation

$$\text{Total cost} = 25 + 1.25 F_{A0} + F_{A0} \times 1.$$

400 FF

$$\text{Total Profit} = 5F_R - 25 - 2.25 F_{A0}$$

400

CSTR

$$\frac{V}{F_{A0}} = \frac{x_A}{-r_A} = \frac{x_A}{5C_{A0}(1-x_A)}$$

$$\begin{aligned} -r_A &= (k_1 + k_2) C_A \\ &= (1+4) C_A \\ &= 5 C_{A0} (1-x_A) \end{aligned}$$

$$F_R = \frac{4}{5} F_{A0} x_A$$

F<sub>A0</sub>

$$\phi = \frac{r_R}{r_S + r_R} = \frac{4 C_A}{4 C_A + C_A} = \frac{4}{5}$$

$$C_{A0} = 1$$

$$\frac{V}{F_{A0}} = \frac{x_A}{5 C_{A0}(1-x_A)}$$



$$\rightarrow \frac{(1-x_A)}{x_A} = \frac{F_{A0}}{5 V C_{A0}} = \frac{F_{A0}}{100}$$

$$\frac{L - i X_A + X_A}{X_A} = \frac{F_{AO} + 100}{100}$$

$$X_A = \frac{100}{100 + F_{AO}}$$

$$P = P_{\text{no fuel}} = 5F_R - 25 - 2.25 F_{AO}$$

$$= 5 \left( \frac{4}{5} F_{AO} X_A \right) - 25 - 2.25 F_{AO}$$

$$= 5 \left( \frac{4}{5} F_{AO} \frac{100}{100 + F_{AO}} \right) - 25 - 2.25 F_{AO}$$

$$\frac{\partial P}{\partial F_{AO}} = 0 = \frac{400(F_{AO} + 100) - F_{AO}}{(F_{AO} + 100)^2} - 0 - 2.25 = 0$$

$$400(F_{AO} + 100) - F_{AO} = 2.25(F_{AO} + 100)^2$$

$$400 \times \frac{100}{(F_{AO} + 100)^2} = 2.25$$

$$(F_{AO} + 100)^2 = \frac{40000}{2.25} = 17777$$

$$F_{AO} = 33.33$$

$$X_A = \frac{100}{F_{AO} + 100} = 0.75$$

fed to reactor.

$+ k_2) C_A$

$(+ 4) C_A$

$5 C_{AO} (1 - X_A)$

# KID FUK KNOWN MIXING, WINDING -

Example : CSTR

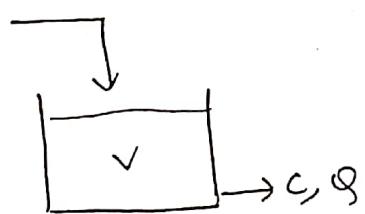
Tracer : Step input junction

$$C_0 Q \Delta \theta - C Q A \theta = V A C$$

$$\frac{dc}{d\theta} = \frac{Q}{V} (C_0 - c)$$

for  $\infty$  time, concentration change: AC.

$C_0, Q$



Again

$C_{pulse}$

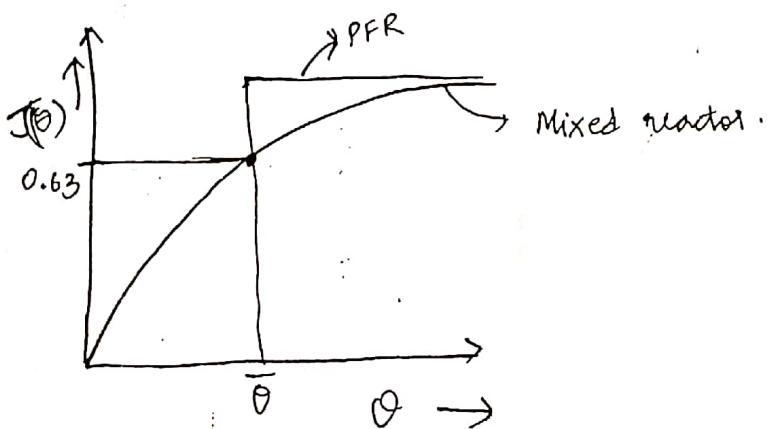


$$\frac{dc}{d\theta} = \frac{1}{\theta} (C_0 - c)$$

$$\int_0^c \frac{dc}{C_0 - c} = \frac{1}{\theta} \int_0^\theta d\theta$$

$$\Rightarrow -\ln \left[ \frac{C_0 - c}{C_0} \right] = \frac{\theta}{\theta}$$

or,  $\left( \frac{c}{C_0} \right)_{step} = J(\theta) = 1 - e^{-\theta/\theta}$



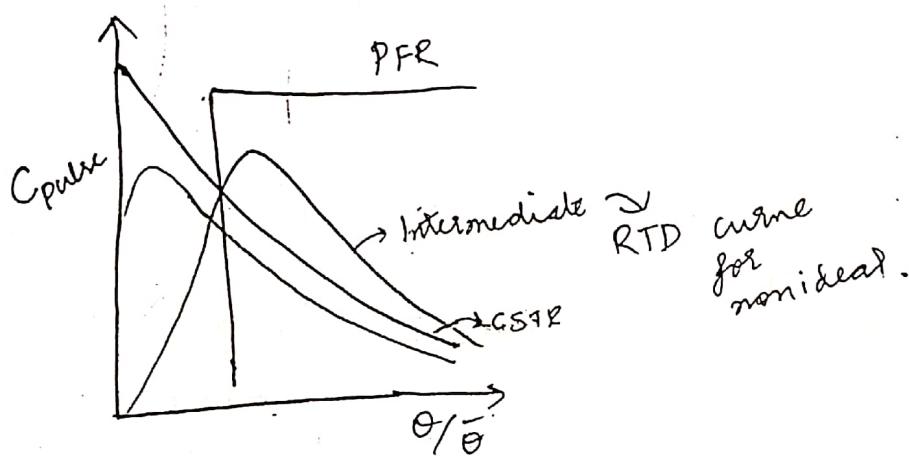
$$J(\theta) = 1 - e^{-\theta/\theta} = 1 - e^{-1} = 0.63$$

$E_{crit}$

$$J'(\theta) = \frac{1}{\theta} e^{-\theta/\theta}$$

Again we have :

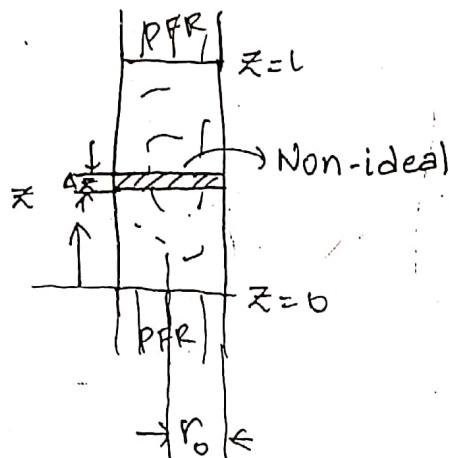
$$\begin{aligned} C_{pulse} &= \frac{M}{Q} J'(\theta) = \frac{M}{Q} \frac{1}{\theta} e^{-\theta/\theta} \\ &= C_0 \Delta t_0 \frac{1}{\theta} e^{-\theta/\theta} \end{aligned}$$



$$E_{avine} = \frac{C_{pulse}}{\int_0^\infty C_{pulse} d\theta}$$

JM  
Smith

# CLOSED VESSEL



Do mole balance  
on the strip:

shell balance

$$\left[ \left( -D_L \frac{\partial c}{\partial z} + u c \right) \pi r_0^2 \right]_z \Delta \theta - \left[ \left( -D_L \frac{\partial c}{\partial z} + u c \right) \pi r_0^2 \right]_{z+\Delta z} \Delta \theta \\ = \pi r_0^2 \Delta z \Delta c$$

- At  $z=0$ , stop input. At this boundary inside and outside will have different conditions.

INITIAL CONDITIONS:  $c = \begin{cases} 0, & z > 0 \text{ for } \theta = 0 \\ c_0, & z < 0 \text{ for } \theta = 0 \end{cases}$

BOUNDARY CONDITIONS: ①  $z=0, \theta \geq 0$

$$-D_L \left( \frac{\partial c}{\partial z} \right)_{z>0} + u(c)_{z>0} = u c_0$$

$$-D_L \left( \frac{\partial c}{\partial z} \right)_{>0} + u(c)_{>0} = u c_0$$

$>0 \rightarrow$  sign used to describe inside the reactor.

②  $z=L, \theta \geq 0$

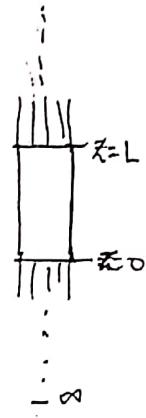
$$\frac{dc}{dz} = 0$$

(With these conditions, it is not possible to solve)

transpiration various ...

$$C^* = \frac{C}{C_0} \quad \alpha = \frac{z - u\theta}{\sqrt{4D_L \theta}}$$

$$\boxed{\frac{d^2 C^*}{d\alpha^2} + 2\alpha \frac{dC^*}{d\alpha} = 0}$$



Boundary conditions :  $C = C_0$  at  $z = -\infty$   
 $C = 0$  at  $z = \infty$

From this we get :

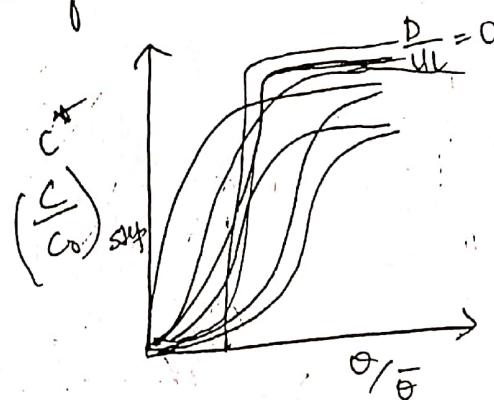
$$C^* = \begin{cases} 0, & z = \infty \\ 1, & z = -\infty \end{cases}$$

$$C^*_{z=L} = \left(\frac{C}{C_0}\right)_{\text{step}} = \frac{1}{2} \left[ e^{-\operatorname{erf}\left(\frac{1}{2} \sqrt{\frac{4L}{D_L}} \frac{1-\theta/\bar{\theta}}{\sqrt{\theta/\bar{\theta}}}\right)} \right]$$

ie and

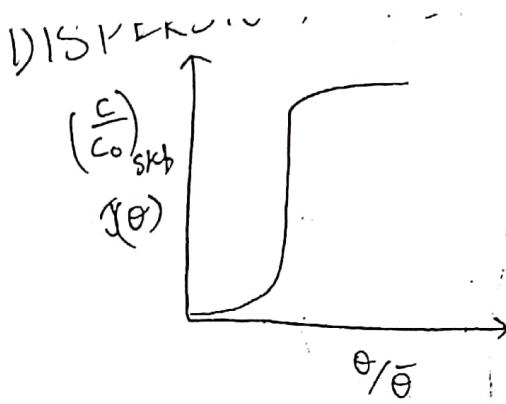
$\frac{D_L}{UL}$  = dispersion number

varying the dispersion number, we will get series of curves of  $C^*$  vs  $\theta/\bar{\theta}$   $\rightarrow$  DISPERSION MODEL



we  $\Rightarrow$  inside

is, if is



If the plot is now ...  
it is close to PFR,

$$\frac{D_L}{UL} = 0$$

0.1, 0.2 → Non-Ideal types-

0.001  
very close

we can

directly use

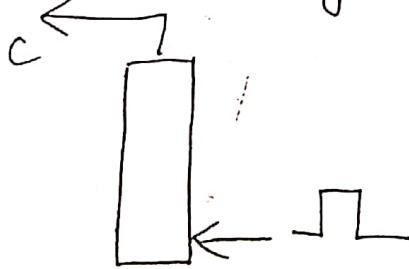
PFR equation

Unknown reactor

RTD plot :-  
for particular  $\frac{D_L}{UL}$  value,  
Expansion of  
Expression → conversion from  $\frac{D_L}{UL}$

## CONVERSION FROM RTD :-

- RTD is already determined.



(mean concentration of)

$$\left( \begin{array}{l} \text{mean concentration} \\ \text{of Reactant} \\ \text{at the outlet} \end{array} \right) = \sum_{\text{all element}} \left[ \begin{array}{l} \text{Concentration of Reactant} \\ \text{remaining in an element} \\ \text{between } t \text{ and } t + \Delta t \end{array} \right] \left[ \begin{array}{l} \text{fraction of exit stream} \\ \text{of stream age between } t \\ \text{and } t + \Delta t \end{array} \right]$$

For 1st

$\bar{C}_A$

$\bar{\bar{C}}_A$

For  
Differ

E

-2

$$\bar{C}_A = \int_{t=0}^{\infty} C_{A, \text{element}} E dt \rightarrow \text{From denegrief (some Q'8)}$$

As per JM Smith book:

$$\bar{C}_A = \int_0^{\infty} C \cdot dJ(\theta)$$

$$\bar{C}_A = \int_0^{\infty} C \cdot J(\theta) dt$$

For 1st Order Reaction:

$$C_{A, \text{element}} = C_{A0} e^{-kt}$$

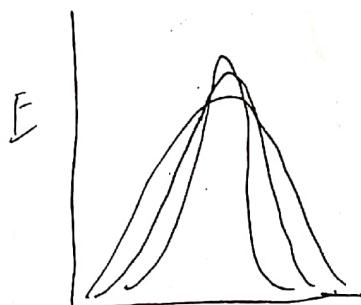
$$\bar{C}_A = C_{A0} \int_0^{\infty} e^{-kt} E dt$$

$$= C_{A0} \sum e^{-kt} E \Delta t$$

$$\bar{X}_A = \frac{C_{A0} - \bar{C}_A}{C_{A0}}$$

From average concentration we can find average conversion.

For different curves, calculate Variance.



$$\begin{aligned} \text{Variance} &= \sigma^2 \\ &= \int_0^{\infty} (t - \bar{t})^2 C dt \\ &\quad \boxed{\int_0^{\infty} C dt} \end{aligned}$$

$$\begin{aligned} \sigma^2 &= \frac{\int_0^{\infty} t^2 C dt}{\int_0^{\infty} C dt} - \bar{t}^2 \approx \frac{\sum (t_i - \bar{t})^2 C_i \Delta t_i}{\sum C_i \Delta t_i} \end{aligned}$$

- $C$  vs  $t$  is available at regular intervals.

$$\sigma^2 = \frac{\sum t_i^2 c_i \Delta t_i}{\sum c_i \Delta t_i} - \bar{t}^2$$

- $C$  vs  $t \rightarrow$  different concentration recorded at the exit.

$C$	0.01	0.05	0.08	
$t$	5	10	15	20
	25	30	35	

or,  $\sigma^2 = \int_0^\infty t^2 E dt - \bar{t}^2$

$$\sigma^2 = \sum t_i^2 E_i \Delta t - \bar{t}^2$$

$$\sigma_\theta^2 = \frac{\sigma^2}{\bar{t}^2}$$

$$\sigma_\theta^2 = \frac{2D}{UL} - 2 \left( \frac{D}{UL} \right)^2 \left( 1 - e^{-\frac{UL}{D}} \right)$$

Steps :-

① E curve

② avg Residence time

③  $\sigma^2$

④  $\sigma_\theta^2$  ( $\frac{\sigma^2}{\bar{t}^2}$ )  $\rightarrow$  Normalized variance.

⑤  $\sigma_\theta^2 \rightarrow \frac{D}{UL}$

⑥ By trial & error method  $\rightarrow$  we can get

$\frac{D}{UL} \rightarrow$  dispersion no -

Soln:

Assumption

-  $r_A$  =

(rate is  
negl)

inf

$F_{AO}$

$F_A$

$F$

(Q) At 953 K, the conversion number  $n \rightarrow 3R$  is same over a solid catalyst of 2 mm. size. The rate equation is :  $r_A' = (0.167 \text{ lit/min g cat}) \cdot CA$

Feed containing 50% A and 50% inert is forced through the bed at 8.33 mol/min. Design packed bed reactor to be used under 5 atm. pressure 953 K isothermal condition for 90% conversion.

$$P_S = 2 \text{ gm/cm}^3$$

catalytic reactor design



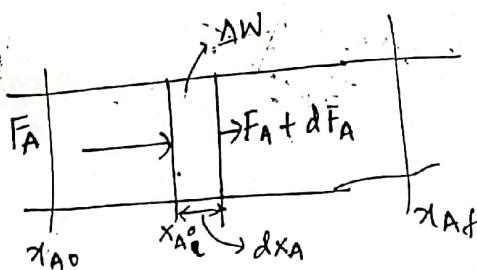
Assumption: Plug flow behavior

$$\epsilon_{AO} = 0.5$$

$$CA = \frac{CA_0 (1-x_A)}{(1+\epsilon_A x_A)}$$

$$r_A' = \frac{1}{W} \frac{dCA}{dt} = 0.167 \frac{\text{lit}}{\text{min.g cat}} \cdot CA$$

(rate is per gm of catalyst is directly write in terms of weight)



input = output + rate of disappearance + accumulation

$$F_{AO} (1 - x_{A\text{in}}) = F_{AO} (1 - x_{A\text{out}}) + (-r_A' \Delta W)$$

$$F_{AO} (x_{A\text{out}} - x_{A\text{in}}) = -r_A' \Delta W$$

$$F_{AO} dx_A = -r_A' dW$$

$$\boxed{-r_A' = F_{AO} \left( \frac{dx_A}{dW} \right)} \quad \text{mole balance}$$

$$C_{AO} = \dots$$

$$\epsilon_B = \dots$$

$$\Rightarrow 1 - \dots$$

$$\Rightarrow 1$$

$$\Rightarrow$$

$$V_S = \dots$$

$$W:$$

$$\bar{F}_{AO} = \dots$$

$$W = \dots$$

$$V_S = \dots$$

$$V_R = \dots$$

Graphical

(1) Start with mole balance

(2) Get the equation

(3) Substitute rate equation

$$W = F_{AO} \int_{x_{AO}}^w \frac{dx_A}{-r_A}$$

$$-r_A' = K \frac{C_{AO}(1-x_A)}{1 + \epsilon_A x_A}$$

$$F_{AO} dx_A = -r_A' dw$$

$$= \frac{F_{AO}}{\epsilon_A}$$

$$F_{AO} \frac{dx_A}{dw} = K \frac{C_{AO}(1-x_A)}{(1 + \epsilon_A x_A)}$$

$$\int dw = \frac{F_{AO}}{K C_{AO}} \int_0^{x_{AF}} \frac{1 + \epsilon_A x_A}{1 - x_A} dx_A$$

can we  
solve  
analytically  
graphically

$$\tau' = \frac{W C_{AO}}{F_{AO}} = \frac{1}{K} \left[ (1 + \epsilon_A) \ln \frac{1}{1 - x_{AF}} - \epsilon_A x_{AF} \right]$$

$$\tau' = \frac{W C_{AO}}{F_{AO}}$$

→ space time for  
catalytic reactor

$$\frac{g \cdot \text{min}}{\text{litre}}$$

$$\therefore \tau' = \frac{W C_{AO}}{F_{AO}} = \frac{1}{0.167} \left[ (1 + 1) \ln \frac{1}{1 - 0.5} - 0.9 x_1 \right]$$

$$\tau' = \frac{W C_{AO}}{F_{AO}} = 22.185 \frac{g \cdot \text{min}}{\text{litre}}$$

$$C_{AO} = \frac{P_t \times Y_{AO}}{RT} = \frac{5 \times 0.5}{0.082 \times 953} = 0.0319 \text{ moles/litre}$$

$$\epsilon_B = \frac{\text{void volume}}{\text{catalytic Reactor volume}} = \frac{V_v}{V_R}$$

→ we want to know catalytic reactor volume so that we can find length.

$$\Rightarrow 1 - \epsilon_B = 1 - \frac{V_v}{V_R} = \frac{V_R - V_v}{V_v}$$

$$\Rightarrow 1 - \epsilon_B = \frac{\text{catalyst volume}}{\text{reactor volume}} = \frac{V_s}{V_R}$$

$$\Rightarrow V_R = \frac{V_s}{1 - \epsilon_B}$$

$$V_s = \frac{W}{\rho_s}$$

$$W = \frac{F_{AO}}{C_{AO}} \cdot 22.185$$

→ we can find out corresponding value / mass of catalyst for any given rate.

$$F_{AO} = 8.33 \text{ mol/min.}$$

$$W = \frac{8.33}{0.0319} \times 22.185 = 5.793 \text{ kg}$$

( $\rho_s \rightarrow$  any solid density ↓ kilograms)

$$V_s = \frac{5793}{\rho_s} = \frac{5793}{2} = 2896.65 \text{ cc.}$$

$$V_R = \text{reactor volume} = \frac{V_s}{(1 - \epsilon_B)} = \frac{2896.65}{0.5}$$

$$= 5793.3 = 5.793 \text{ litre}$$

Graphically area = 3.75  
 $W = 5.85 \text{ kg}$

(slight difference).

If the rate equation is per unit volume basis:

$$\frac{V_S K C_{A0}}{F_{A0}} = (1 + \epsilon_A) \ln \frac{1}{1 - X_A} - \epsilon_A X_A$$

$$= 4 \ln \frac{1}{1 - X_A}$$

$$F_{A0} \cdot \frac{dX_A}{dV} = -r_A^{(1)} \frac{\text{mol}}{\text{lit min}} \quad (\text{per unit volume of catalyst})$$

$$F_{A0} \cdot \frac{dX_A}{dw} = -r_A^{(1)} \cancel{\frac{\text{mol}}{\text{m}^2 \cdot \text{min}}} \quad (\text{per unit surface area of catalyst})$$

The following values are obtained :-



$$F_{AO} = 10 \text{ kg-mol/hr.}$$

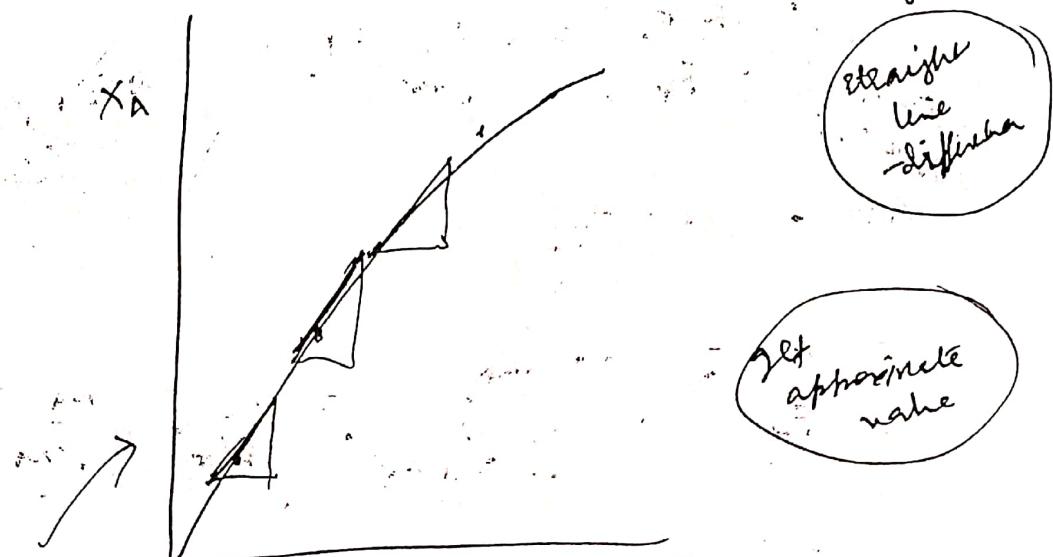
Differential method of analysis : plot  $x_A$  vs.  $w$

$$F_{AO} \frac{dx_A}{dw} = -r_A$$

$$\frac{dx_A}{d\left(\frac{w}{F_{AO}}\right)} = -r_A$$

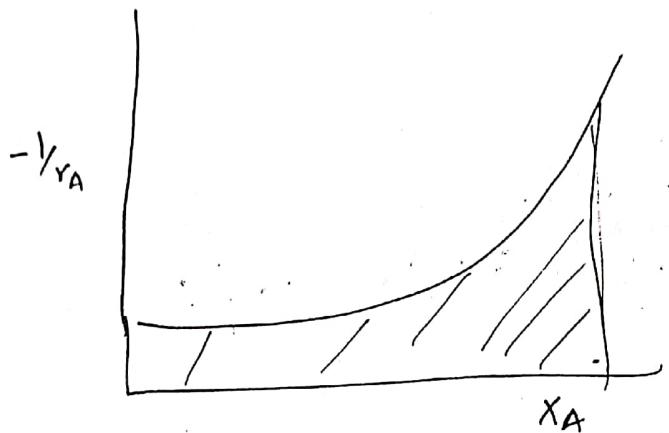
$w/F_{AO}$	0.1	0.2	0.3	0.4	0.5	0.6	0.7
$x_A$	0.12	0.2	0.27	0.33	0.37	0.41	0.44
$-r_A$	0.12	0.2	0.27	0.33	0.4	0.44	0
$-r_A$	0.9	0.975	0.63	0.525	0.362	0.195	0.175
$-r_A$							

reaction  
is  
integral



Find  
slope at  
different  
points.

$w/F_{AO}$



$$-\frac{r_A}{X_{A0}}$$

$$\text{Area} = 0.865 \quad W = 226. \text{ kg}$$

by integral method

Assume 1<sup>st</sup> order

$$\frac{W}{F_{A0}} = \int_0^{X_A} \frac{k dX_A}{K C_{A0} (1-X_A)} = \frac{1}{K C_{A0}} \ln \left( \frac{1}{1-X_A} \right)$$

~~0. lever rule  
1/4 additn~~

18, 19  
calculus  
molar  
law

$$W \left( \frac{K C_{A0}}{F_{A0}} \right) = \ln \frac{1}{(1-X_A)} = P_1$$

W vs P plot is  
not straight line.

correlation coefficient 0.7

Assume 2<sup>nd</sup> order

$$\frac{W}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{K C_{A0}^2 (1-X_A)^2} = \frac{1}{K C_{A0}^2} \left[ \frac{X_A}{1-X_A} \right]$$

$$W \left( \frac{K C_{A0}^2}{F_{A0}} \right) = \frac{X_A}{1-X_A} = P_2$$

correlation coefficient 0.998

$$\frac{W}{F_{A0}} = \frac{K C_{A0}^2}{F_{A0}} \left[ \frac{X_A}{1-X_A} \right]$$

$$K C_{A0}^2$$

$$W = ?$$

$W$	1	2	3	4	5	6	fr coefficient
$\frac{m}{1-x_A}$	0.128	0.223	0.3147	0.4	0.462	0.527	0.598
$\frac{x_A}{1-x_A}$	0.136	0.25	0.369	0.452	0.567	0.695	0.785

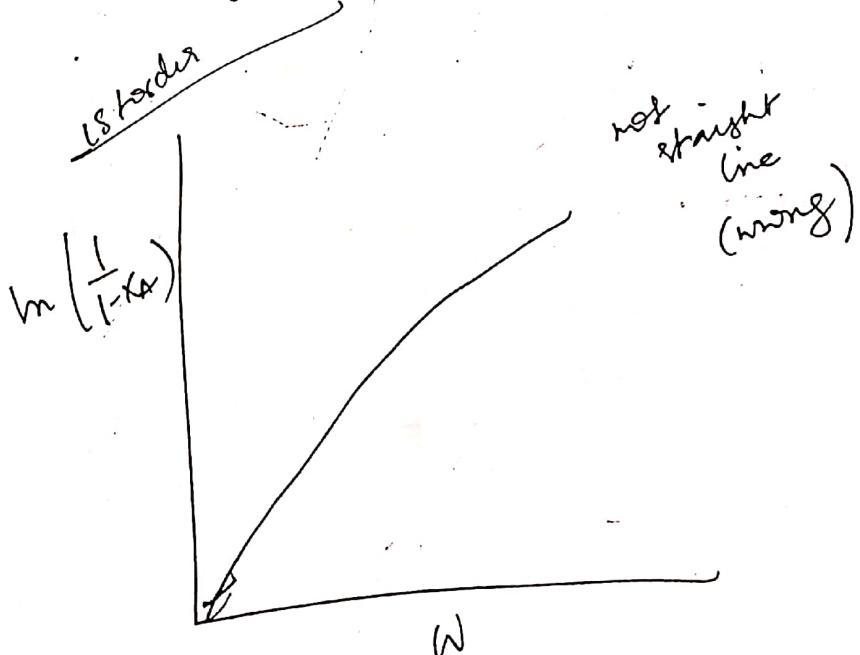
fitted model — second order kinetics

$$\frac{k C_{AO}^2}{F_{AO}} = 0.1158$$

$$k C_{AO}^2 = +.158$$

$$W = \frac{x_A}{1-x_A} \cdot \frac{F_{AO}}{k C_{AO}^2} = \frac{0.4}{0.6} \times \frac{400}{1.158}$$

$$= 230.2 \text{ kg}$$



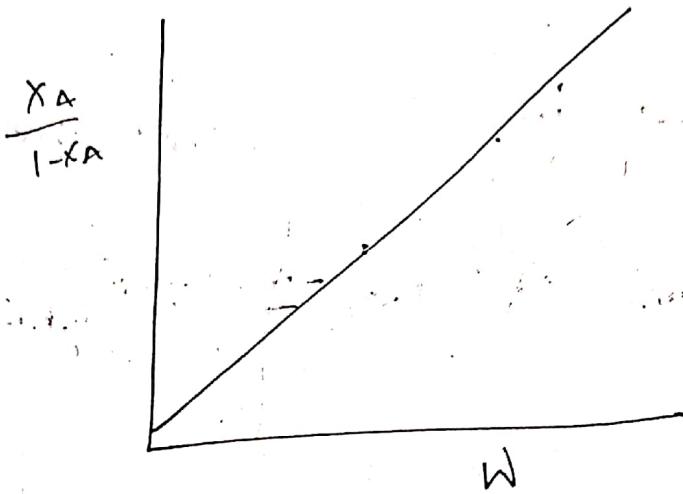
a)

vs P plot is  
not straight line.

$\left[\frac{x_A}{1-x_A}\right]$

relation coefficient  
0.998

denominational  
Chapter



2nd order

straight  
line  
curve

- 1) Read chapter 5 (only mole balance)  
Q's will be from catalytic reactions. (No homogenous)
- 2) Multiple reactions,  
multiple reactors } Chapter 6
- 3) optimization
- 4) Parallel reactions Chapter 7
- 5) RTD. Chapter 9 → non ideal reactor

K

For R =

T, P effect

CKCap is same

enemphie  
Technik

denmark  
chapter 6/13

conversion  $\frac{2}{3}$

$2A \rightarrow 2R$

$$R = 1$$

$$-r_A = k C_A^2, \epsilon_A = 0$$

$$\frac{k C_{A_0} z}{R+1} = \frac{C_{A_0} (C_{A_0} - C_{A_f})}{C_A f (C_{A_0} + R C_{A_f})}$$

$$K_C = \frac{2 (C_{A_0} - C_{A_f})}{C_{A_f} (C_{A_0} + C_{A_f})} = \frac{2 (C_{A_0} - C_{A_0} + C_{A_0} x_A)}{C_{A_0} (1-x_A) (C_{A_0} + x_A (C_{A_0} x_A))} \\ = \frac{2 x_A}{(1-x_A) C_{A_0} (2-x_A)}$$

$$C_{A_0} K_C = \frac{2 x_A}{(1-x_A) (2-x_A)}$$

$$K_C C_{A_0} = 3$$

for  $R=0$  PFR

$$\frac{V}{F_{A_0}} = \int_0^{X_A f} \frac{dX_A}{k C_{A_0}^2 (1-X_A)^2}$$

$$2K C_{A_0} = \int_0^{X_A f} \frac{dX_A}{(1-X_A)^2} = \frac{1}{1-X_A} \Big|_0^{X_A} \\ = \frac{1}{1-x_A} - 1 = \frac{x_A}{1-x_A}$$

$2K C_{A_0}$  is  
same

$$3 = \frac{x_A}{1-x_A}$$

$$x_A = 0.75$$

## Assignment 2

$$F_{AD} = 20000 \times 0.1 = 200 \text{ kg/day}$$

$$F_r = F_{A0} \times A$$

$$V_i = \frac{F_{AO} X_A}{K C_A} = \frac{200 X_A}{0.25 \times 24 \times 0.01 (1-X_A)}$$

$$= \frac{20000}{6} = \frac{XA}{1-XA}$$

$$P = 3 \times 10^6 X_A - 649519 \frac{X_A^{1/2}}{(1-X_A)^{1/2}} - 3 \times 10^5$$

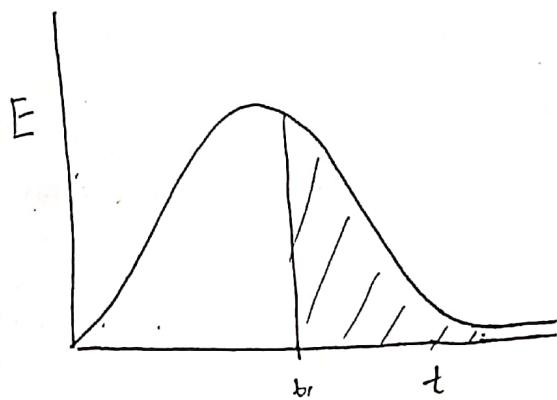
find  $x_A$

By trial and

$$\frac{dP}{dX_A} = 3 \times 10^6 - 64$$

Find someone for  
magazine project

# E CURVE



$$E = J'(\theta) = \frac{dJ(\theta)}{d\theta}$$

What fraction is older than  $t_1$  minute?

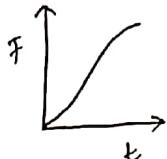
$$\int_{t_1}^{\infty} E dt = 1 - \int_0^{t_1} E dt$$

Fractional Age distribution

$$\int_0^{\infty} E dt = 1$$

- time vs Concentration - given  
calculate E curve, F curve.

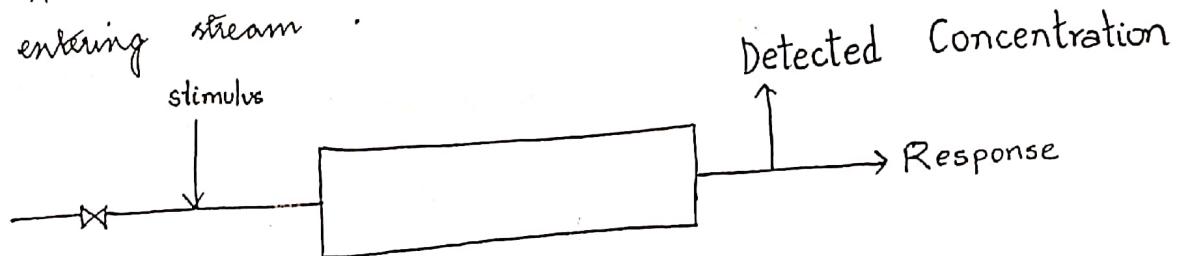
F CURVE →



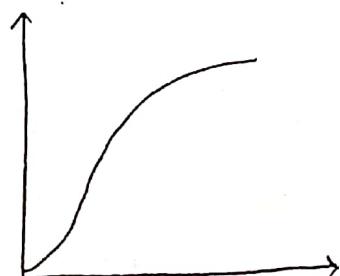
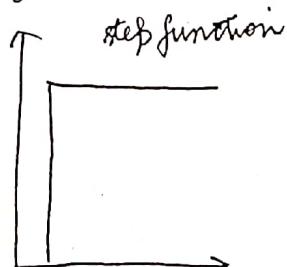
$J(\theta)$  vs  $\theta$  curve is F

## STIMULUS RESPONSE METHOD

A stimulus is a trace input which is added to the inlet of entering stream.



Response is the measured output function w.r.t to stimulus  
If we add a step input, the output we will get immediately.  
ratio of Output by Input



If we get the same plot as input, then it is a ideal reactor, PFR.

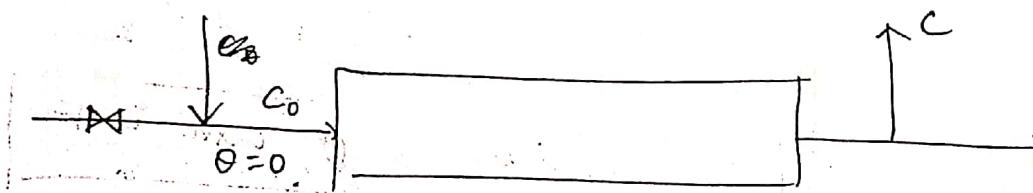
We have to measure how much it has deviated.

Then finding the stimulus we have to calculate RTD.

### ~~STEP INPUT~~

At  $\theta = 0$ , all molecules are marked to distinguish them from the molecules entered prior to  $\theta = 0$ .

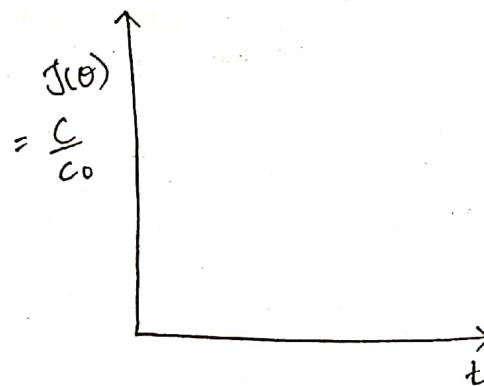
- \* During RTD, there is ~~is~~ no reaction (ASSUMPTION).
- \* Now its marked - measure the concentration at the exit.
- \* Eg: Initial conc.  $C_0$



$$C_0 \cdot J(\theta) = C$$

$$J(\theta) = \frac{C}{C_0}$$

∴ F-curve :  $J(\theta) = \frac{C}{C_0}$



We know the initial concentration.

$$C_0 = 5$$

$C$	0	4	7	9	11	11.5	12
$\theta$	0	10	20	30	40	50	60
min	0	4/5	7/5	9/5	11/5	11.5/5	12/5
$C/C_0$	0	4/5	7/5	9/5	11/5	11.5/5	12/5

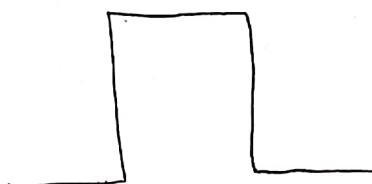
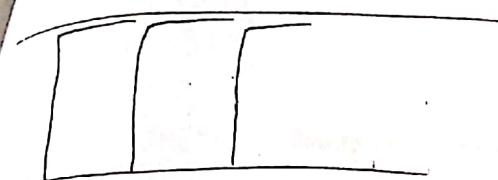
Observe the concentration at outlet &

then ~~plot~~ plot  $C$  vs  $\theta$  &

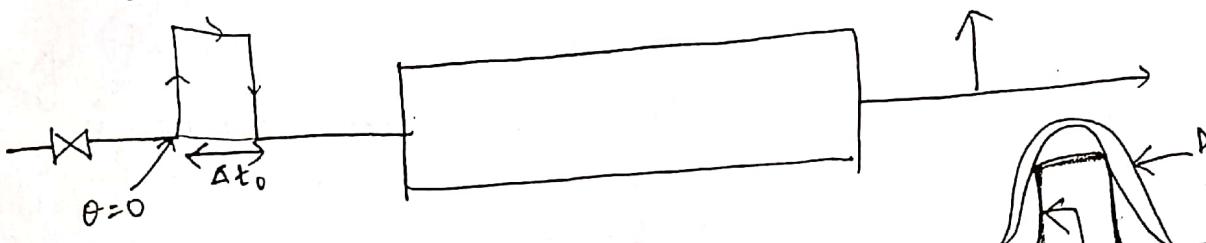
... come.

pulse input  $\rightarrow$  We get E curve & F curve directly - we need to calculate -

We get C curve



Stimulus



Deviation non ideal.

close to PFR

Non-ideal - we have to predict the conversion.  $\rightarrow$  how much non ideality

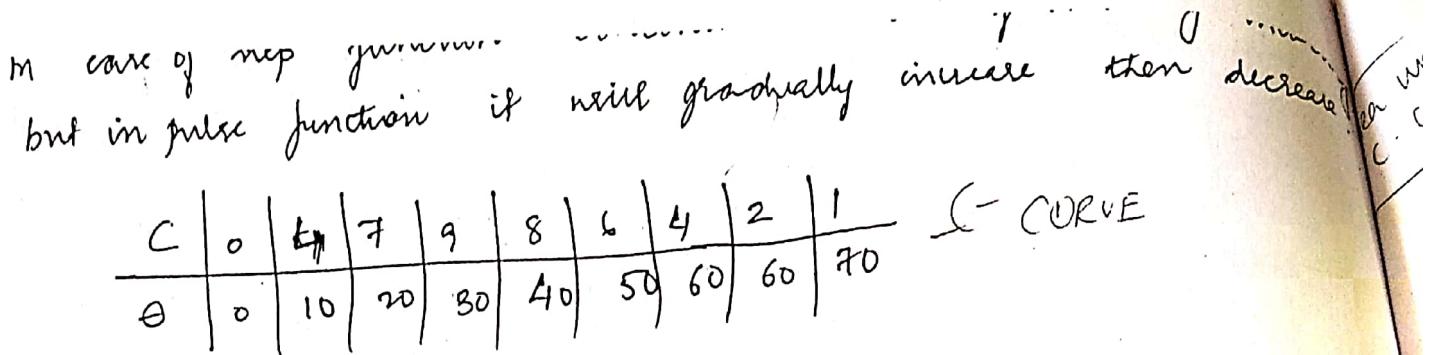
From the flow behavior  $\rightarrow$  we will see the RTD then we will compare with standard value & calculate conversion.

If all molecules are marked for a short span of time say  $\Delta t_0$ , at  $\theta = 0$ , the total concentration for marked molecules:

$$M = C_0 \Delta t_0$$

( Hypodermic syringe  $\rightarrow$  using this ethylene is injected (for volume) and we get pulse input by injecting for short amount of time).

$$C = \begin{cases} 0, & \text{for } t < 0 \\ C_0, & 0 < t < \Delta t_0 \\ 0, & t > \Delta t_0 \end{cases}$$



At the outlet  $C$  vs  $\theta$  curve is the response curve.  
No. of molecules leaving in the period  $\theta$  and  $\theta + \Delta\theta$  is  $dJ(\theta)$ .  
Differential fraction  $dJ(\theta)$  will leave the reactor between  $\theta$  and  $\theta + \Delta\theta$ .

$dJ(\theta) = J'(\theta) \Delta\theta$  → Within  $\Delta\theta$  this much fraction is coming out.

Thus we can write: ( $M$  = total concentration)

$$M J'(\theta) \Delta\theta = C Q \Delta\theta$$

$Q$  = volumetric flow rate

$C$  = concentration.

$$J'(\theta) = \frac{C_{pulse} \cdot Q}{M} = E$$

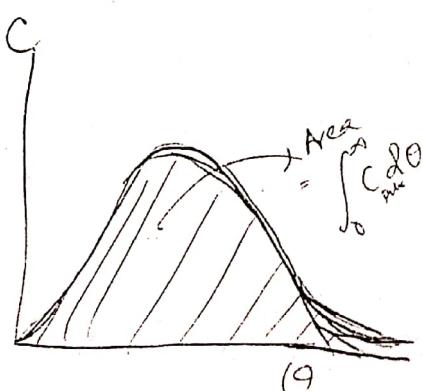
\*  $E$  is still unknown because  $M$  is unknown  $\rightarrow$

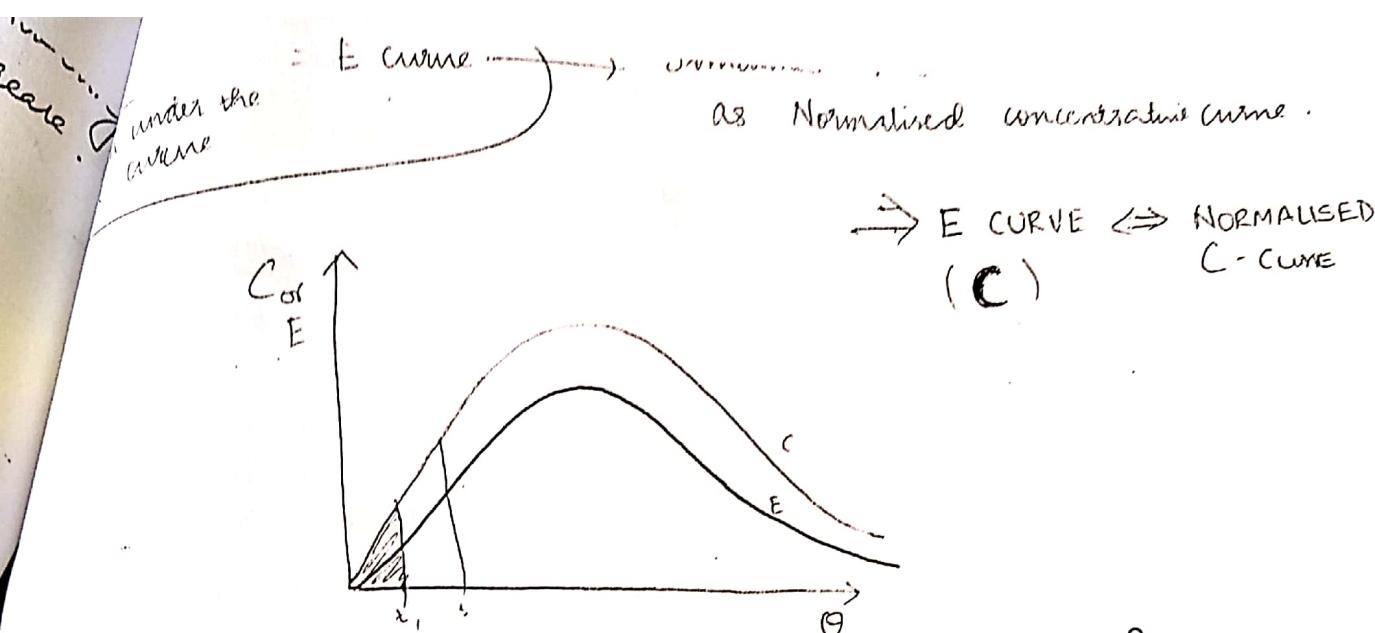
$M$  is very difficult to measure for such small  $\theta$ .

∴ It is calculated in REVERSE process.

$$M = Q \int_0^\infty C_{pulse} d\theta$$

$$E = \frac{C_{pulse} \cdot Q}{Q \int_0^\infty C_{pulse} d\theta}$$





Using Pulse inputs  $\rightarrow$  how to find F curve?

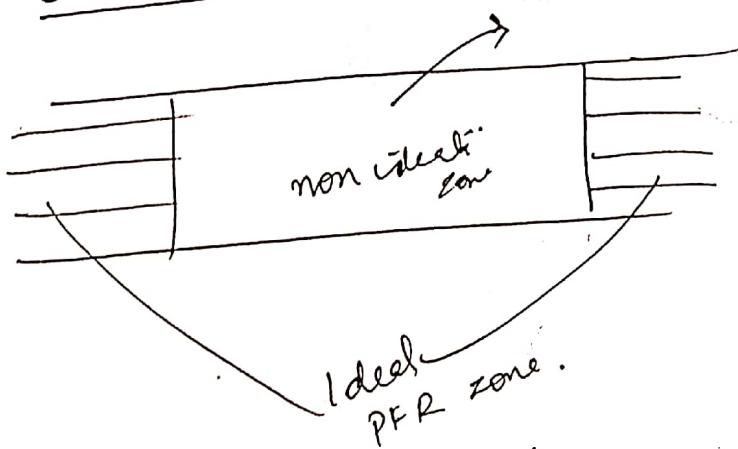
$$E = \frac{C_{pulse}}{\int_0^{\infty} C_{pulse} d\theta}$$

$$F = \frac{\int_0^t C_{pulse} d\theta}{\int_0^{\infty} C_{pulse} d\theta}$$

Verenigd  
Chapters 9

For all this analysis : ASSUMPTION :

$\rightarrow$  ~~PFR before and after PFR~~ (ideal  $\rightarrow$  before & after)  
CLOSED VESSEL      Analyze only for non ideal behavior



Response:  
 Response : curve for a pulse input is

$$E = \frac{dF}{d\theta}$$

derivative of the ~~same~~ response  
 same of step input .

$$E = \frac{C_{\text{pulse}}}{\int_0^\infty C_{\text{pulse}} d\theta}$$

$$= \frac{C_{\text{pulse}}}{M}$$

$$F = \frac{\int_0^\infty C_{\text{pulse}} d\theta}{\int_0^\infty C_{\text{pulse}} d\theta}$$

$$f = \frac{1}{M} \int_0^t C_{\text{pulse}} d\theta$$

(Derivation in  
JM Smith.)

$$J'(\theta) \Big|_{\text{step}} = \frac{d J(\theta)}{d\theta} = \frac{d \left( \frac{c}{c_0} \right)_{\text{step}}}{d\theta}$$

$$\frac{C_{\text{pulse}} Q}{M} = \cancel{Q} J(\theta)$$

$$\text{For finite : } Q(\theta) \approx \frac{M}{Q} J(\theta) = C_{\text{pulse}}$$

$$C_{\text{pulse}} = \frac{c_0}{Q_{\text{pulse}}} \frac{Q \Delta t_0}{Q} J(\theta)$$

$$\frac{C_{\text{pulse}}}{c_0} = \Delta t_0 J(\theta) = \Delta t_0 \frac{d \left( \frac{c}{c_0} \right)_{\text{step}}}{d\theta}$$

$$\boxed{\frac{C_{\text{pulse}}}{c_0} \propto \frac{d}{d\theta} J(\theta)_{\text{step}}}$$

1st order liquid phase reaction is to be carried out in a reactor vessel which is ~~suspected~~ <sup>pure input</sup> to be non-ideal. A trace input of delta function has given the following response. What conversion would you expect in this reactor? A mixed reactor with the same space time of the above reactor gives 82% conversion.

$t$	0	10	20	30	40	50	60	70	80
tracer conc	0	3	5	5	4	2	1	0	0

If the reactor is represented with dispersion and tank-in-series model what conversion would you expect?

Dispersion model, Tank in series model

① calculate avg residence time  $\rightarrow$  summation method.

$$\bar{t} = \frac{\sum t_i C_i A t_i}{\sum C_i A t_i} = \frac{800 \times 10}{200} = 40 \text{ sec}$$

$A t_i = 10$

$t$	$C$	$t_i C_i$	$e^{-K_{t,i} t_i}$
10	0	0	0
20	3	60	0.3076
30	5	150	0.1641
40	5	200	0.0525
50	4	200	0.0125
60	2	120	0.00216
70	1	70	0.00034
80	0	0	0
		$\sum 800$	$e^{-0.5402}$

For mixed reactor

$$C = X_A = 4.55$$

$$K(1-X_A)$$

$$\frac{K}{C} = 4.55$$

1st order

$$C = 40 \therefore K = 0.1138 \text{ mc}^{-1}$$

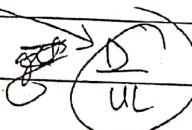
(2) calculate  $\sigma^2$  &  $\sigma_0^2$ 

$$\sigma^2 = \left( \frac{\sum t_i^2 \cdot C_i A t_i}{\sum C_i A t_i} \right) - \left( \bar{t} \right)^2 = \frac{358000 - 40^2}{200}$$

$$\sigma^2 = 190$$

$$\frac{\sigma_0^2}{\bar{t}^2} = \frac{\sigma^2}{40^2} = \frac{190}{40^2} = 0.12$$

(3) Assume closed vessel.



$$\frac{2D}{UL} = \sigma_0^2$$

$$\frac{D}{UL} = 0.06$$

$$\sigma_0^2 = \frac{2D}{UL} - 2 \left( \frac{D}{UL} \right)^2 \left( 1 - \frac{UL}{D} \right)$$

$$= 2(0.06) - 2(0.06)^2 \left( 1 - e^{-\frac{1}{0.06}} \right)$$

$$= 0.1193$$

$$\frac{D}{UL} = 0.08 \quad \sigma_0^2 = D \cdot 1.472$$

$$\frac{D}{UL} = 0.05 \quad \sigma_0^2 = 0.095$$

$$\frac{D}{UL} = 0.06$$

We are getting stuck  
Juggling

6

$$\frac{C_A}{C_{A0}} = \exp \left[ -kT + (kC)^2 D \right]_{UL}$$

$$= \exp \left( -0.1138 \times 40 + (0.1138 \times 40^2) \times 0.06 \right)$$

$$= 0.0365$$

$$\text{so } X_A = 0.9634 \quad \cancel{\text{Ans}}$$

*dispersion*

CSTR in series model

$$N = \frac{1}{\frac{1}{0.02}} = \frac{1}{0.12} = 8.33$$

$$X_N = 1 - \frac{1}{(1+kC)^N} = 0.9728$$

RTD

$$\bar{C}_A = \int_0^\infty C_{A0} e^{-kt} E dt$$

$$= C_{A0} \left( \sum e^{-kt} C_A(t) \right) = C_{A0} \left( \sum e_C \Delta t_i \right)$$

we can use

E curve

or directly use  
pure unforced

Curve C  
curve

$$\bar{C}_A^{Ati} = 0.5402 \times 10 = 5.402$$

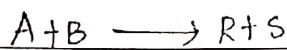
$$\bar{C}_A = \frac{5.402}{200} = 0.027$$

$$X_A = 1 - \frac{\bar{C}_A}{C_{A0}} = 1 - 0.027 = 0.973$$

~~Find my PFR  
if  $q_2 \rightarrow PFR$ . Conclusion of PFR given different values in the PFR vs CSTR.~~

## Assignment 2

(1)



$$C_{A0} = 0.9 \text{ mol/lit.}$$

$$X_A = 0.94$$

$$-r_A = k C_{A0} (1 - X_A)^2$$

$$E_A = 0$$

$$\tau = \frac{C_{A0}}{k C_{A0}^2 (1 - X_A)} \int_0^{X_A} dX_A$$

$$= \frac{1}{k C_{A0}} \int_0^{X_A} \frac{dX_A}{1 - X_A}$$

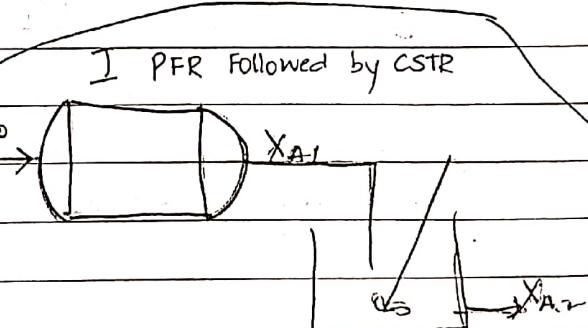
$$= \frac{1}{k C_{A0}} \left[ \ln(1 - X_A) \right]_0^{X_A}$$

$$V = \frac{V_0}{K C_{A0}} \times \frac{0.94}{1 - 0.94} = \frac{17.41}{K}$$

$$\text{Volume of CSTR} = (10V)$$

$$V_m = \frac{174.01}{K} V_0$$

K



$$\frac{V_m}{V_0} = \frac{C_{A0} (X_{A2} - X_{A1})}{-r_2}$$

$$= \frac{X_{A2} - 0.94}{k C_{A0} (1 - X_{A2})^2}$$

PFR, followed by CSTR  
CSTR " " PFR  
2PFR, 2CSTR (J/H sizes)

Optimization Problem, total cost

From CSTR balance

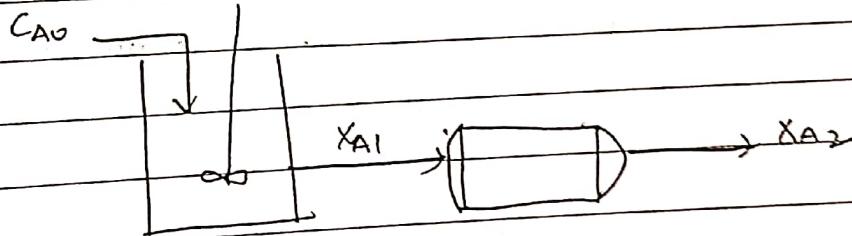
$$\frac{174.1 V_0}{V_0} = \frac{x_{A_2} - 0.94}{0.9 K(1-x_{A_2})^2}$$

$$\Rightarrow x_{A_2} = 0.9836, 1.029$$

$$\Rightarrow x_{A_2} = 0.9836$$

$$\text{Conversion increased by } \frac{0.9836 - 0.94}{0.9836} \times 100 \\ = 4.61\%$$

## II CSTR followed by PFR



$$\tau = \frac{C_{A0}}{K C_{A0}^2 (1-x_{A1})^2} (x_{A1} - x_{A0})$$

$$\tau = \frac{174.1}{K C_{A0}^2 (1-x_{A1})^2} (x_{A1} - x_{A0})$$

$$x_{A1} = 0.923$$

$$\frac{174.1}{K} = \frac{x_{A1} - x_{A0}}{C_{A0}^2 (1-x_{A1})^2}$$

$$x_{A1} = 0.923$$

iii PFR balance :-

$$17.41 C_{A0} = \frac{dX_A}{\sqrt{X_{A1}} (1-X_A)^2}$$

$$X_{A2} = 0.965$$

$$\text{conversion increased by} = \frac{0.965 - 0.94}{0.94} \times 100 \\ = 2.659 \\ = 2.66\%$$

iv CSTR

so 1st arrangement is better

> Step-wise mol balance

If it is 1st order then ? - No change in conversion -

$$C_{A1} = C_{A0}$$

$$1 + k_p t_m$$

$$k_p = \ln \frac{C_{A1}}{C_{A2}}$$

$$C_{A2} = C_{A0} \cdot \frac{e^{-k_p t_m}}{1 + k_p t_m}$$

$$r_p = - \frac{dC_A}{dt_m} \cdot K_p$$

