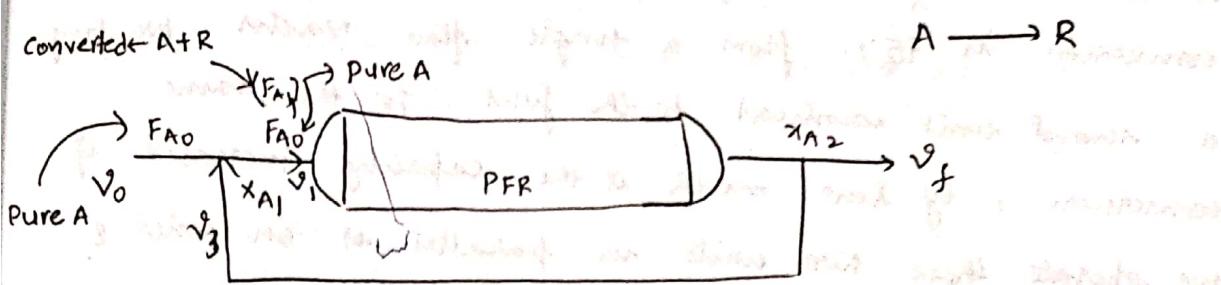


# RECYCLE REACTOR

26/09/19



$$V_3 = R V_f ; F_A0$$

R = Volume of fluid returned to the feed

volume leaving the system

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

$$\frac{V}{F_{A0}} = \int_{x_{A1}}^{x_{A2}} \frac{dx_A}{-r_A}$$

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

- Backmixing of the product stream
- Conversion of the inlet stream changes.
- mole balance  $F_{A0}' \rightarrow$  pure A

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

$$C_{A1} = C_{A0} \left( \frac{1 - \frac{R}{R+1} X_{Af}}{1 + \frac{R E_A X_A}{R+1} X_{Af}} \right) = \frac{F_{A0} (1 + R (1 - X_{Af}))}{V_0 (1 + R (1 + E_A X_A))}$$

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

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

### Question #1

A substance A reacts 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 ?

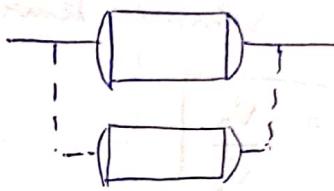
- (a) The reactors are both plug flow  
 (b) The reactors are both mixed flow

#### (a) PFR

# Parallel

For a single reactor

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



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

$$V K C_{AO} = 19 V_1$$

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

$$V K C_{AO} = 19 V_2$$

$$V_1 = V_2$$

$$V_1 + V_2 = 2 V_2$$

# Series

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

Single

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

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

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

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

### (b) MIXED REACTOR

# Parallel

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

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

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

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

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

$$\frac{VK_{AO}}{V_2} = 380 \quad \frac{VK_{AO}}{V_2''} = 380$$

$$V_2' = V_2'' = \frac{VK_{AO}}{380}$$

$$V_2 = 2V_1$$

Q2 Series

$$v = v_1$$

$$C = \frac{x_1}{KC_{AO}(1-x_f)^2} = \frac{380}{KC_{AO}} \quad \boxed{C_1 = C_2}$$

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

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

=> solve for  $x_1$

By trial  $x_1 = 0.8525$

$$C_1 KC_{AO} = 39.18$$

$$\frac{V}{v_2} |KC_{AO} = 39.18 \quad \frac{V}{v_1} \times \frac{v_2}{V} = \frac{380}{39.18}$$

$$\frac{V}{v_1} KC_{AO} = 380$$

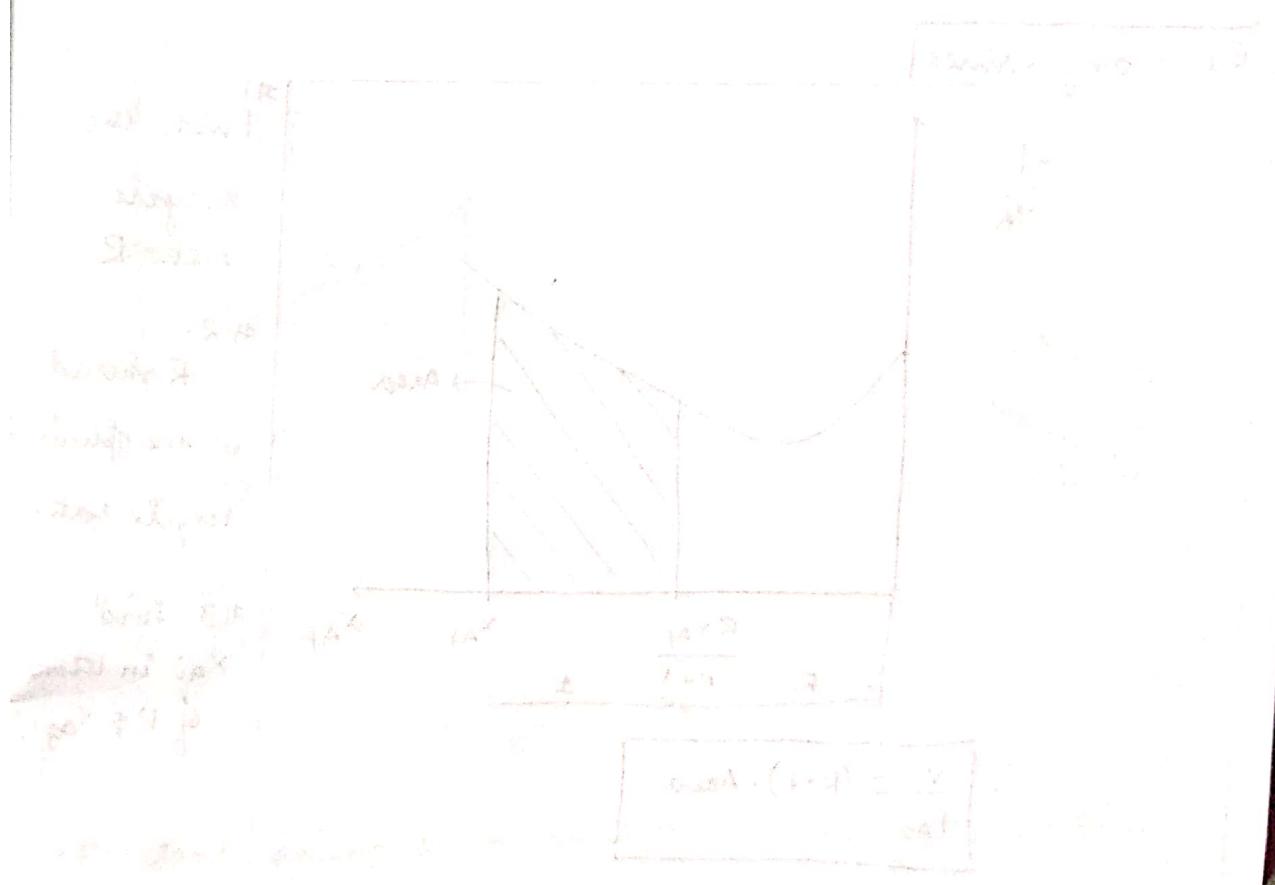
$$\frac{v_2}{v_1} = 9.695 \approx 10$$

### Practice Problem

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.

(slow rate)

- (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?



30/09/19

# Recycle Reactor Design

(TODAY'S LECTURE -  
theory is imp.)

$$\frac{V}{F_{A0}} = R+1 \int_{\frac{R \cdot x_{Af}}{R+1}}^{x_{Af}} \frac{dx_A}{-r_A}$$

GENERAL

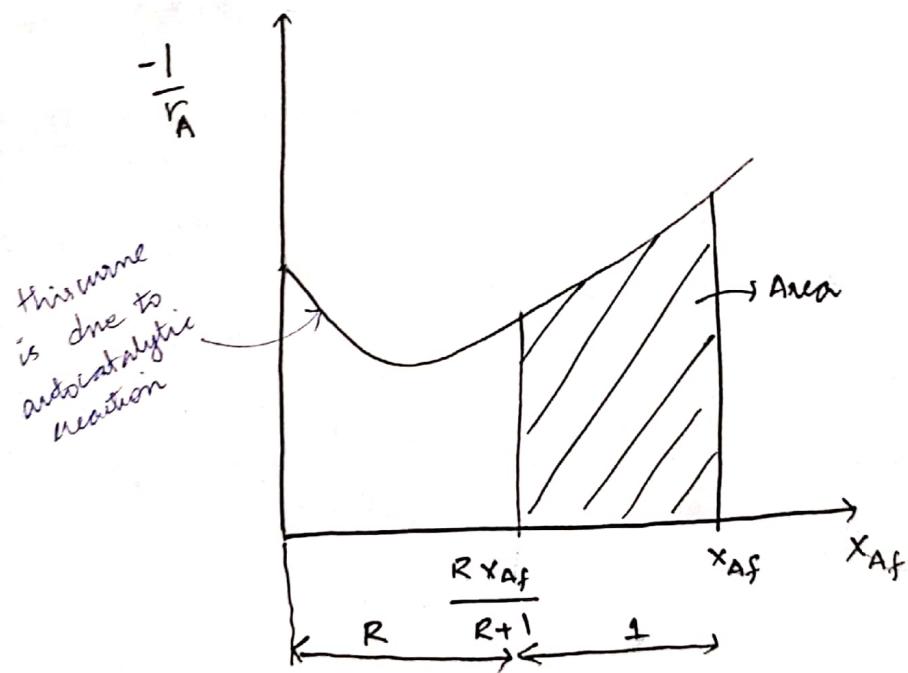
$$\Rightarrow T_R = \frac{C_{AO} V}{F_{AO}} = -(R+1) \int_{\frac{c_{AO} + R c_{Af}}{R+1}}^{c_{Af}} \frac{dc_A}{-r_A}$$

for  $\epsilon = 0$

liq phase  
or  
no inert

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

$E_A$  - any values

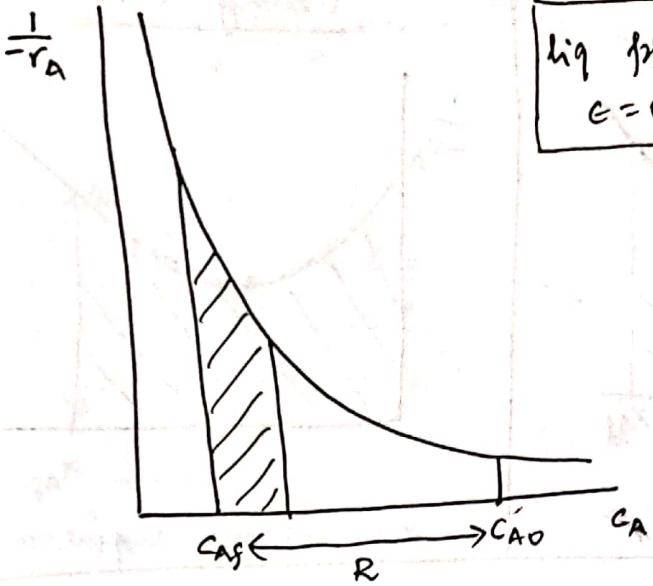


$$\therefore \frac{V}{F_{AO}} = (R+1) \cdot \text{Area}$$

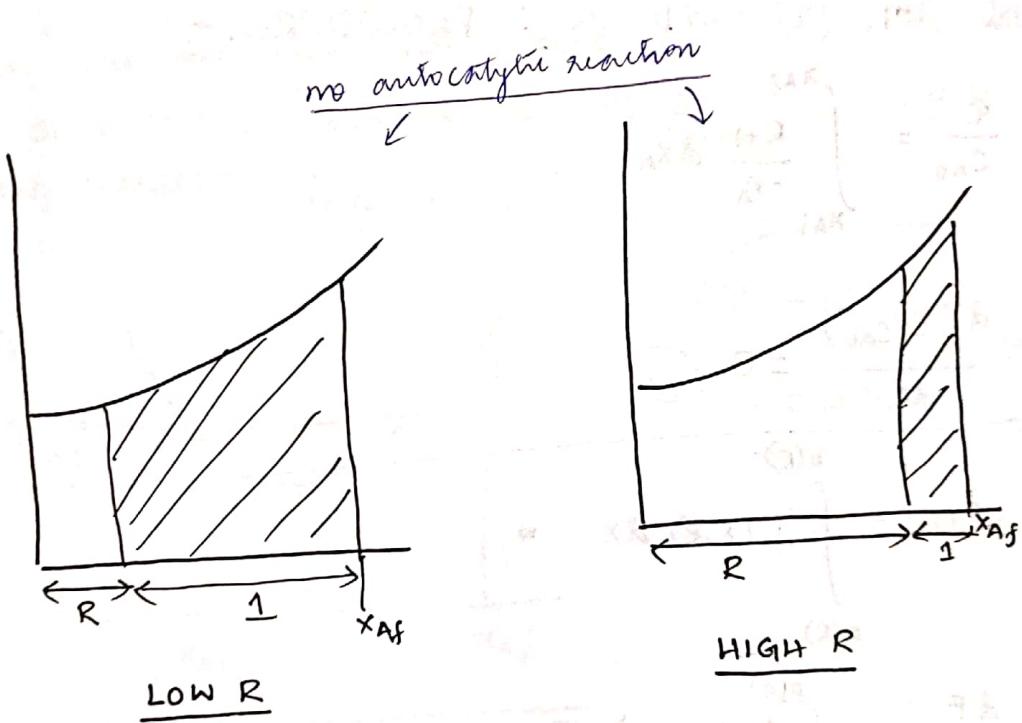
#1 Find the recycle ratio  $R$

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

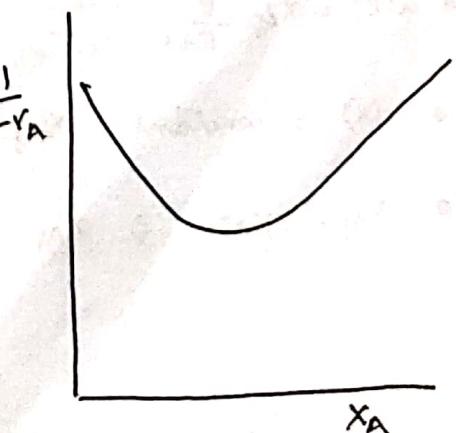
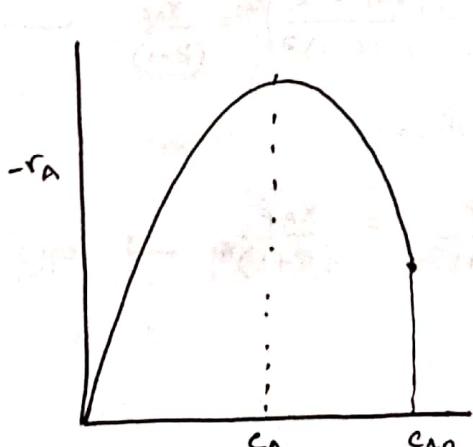
#3: Find  $x_{Ai}$  in term of  $R$  &  $x_{Af}$



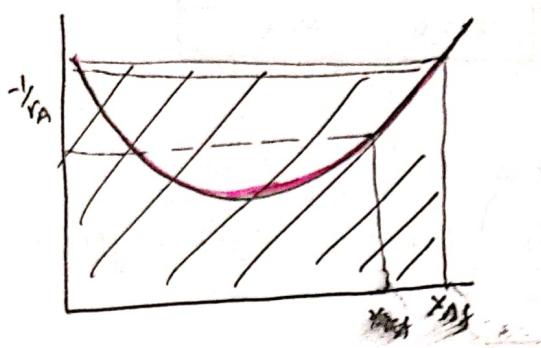
liq phase reaction  
 $E = 0$



- Reactant acting as a catalyst - autocatalytic reaction  
(decreases)  $A + R \rightarrow R + R$

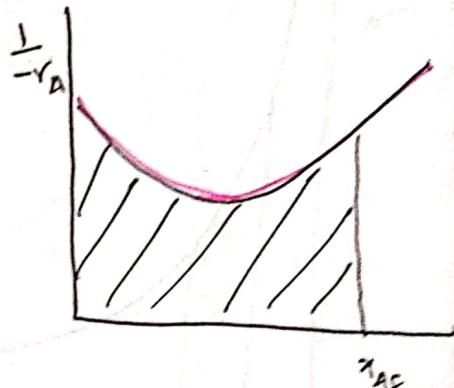


Using CSTR



Large volume required

Using PFR



Less volume required

TO FIND THE OPTIMIZED 'R': PROCEDURE:-

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

$$\#2. \frac{d(C/C_{AO})}{dR} = 0 \rightarrow$$

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

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

Applying the above formula:

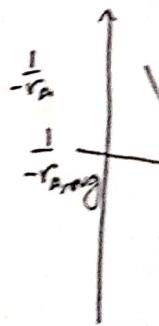
$$a(R) = x_{Af} \frac{R}{R+1}$$

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

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

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

From this  
BE SUCH  
CAN EVA



TO FIND

$A \rightarrow R$

cost of R

Feed rate

$C_M = f$

FIND THE  
RATE

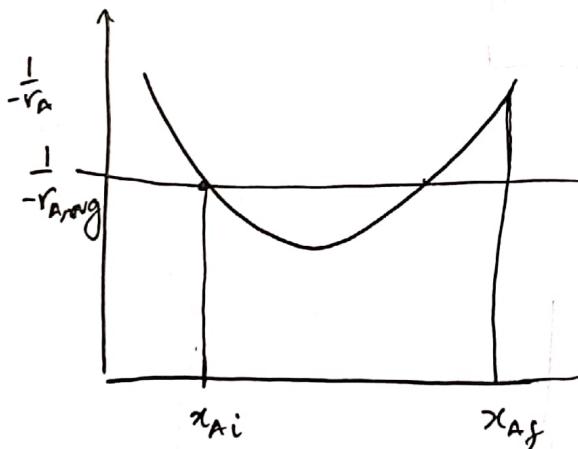
$$\frac{d(\frac{C}{C_{AO}})}{dR} = 0 = \int_{x_{Ai}}^{x_{Af}} \frac{dx_A}{-r_A} + 0 - \frac{R+1}{-r_A} \left| \frac{dx_{Ai}}{dR} \right| - eq(3)$$

Using equation 1, 2, 3 :-

$$\left| \frac{-1}{r_A} \right|_{x_{Ai}} = \frac{\int_{x_{Ai}}^{x_{Af}} \frac{dx_A}{-r_A}}{(x_{Af} - x_{Ai})} \Rightarrow \text{average of } \frac{1}{-r_A}$$

$$= \frac{-1}{r_{A,\text{avg}}}$$

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  $x_{Ai}$ ,  $\frac{1}{-r_A}$  is evaluated.

### To FIND OPTIMUM REACTOR SIZE



cost of Reactant ( $C_{AO}$ ) =  $C_R R_s / K \text{mol}/\text{A}$

Feed rate =  $F_{AO} \text{ kmol}/\text{hr}$

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

FIND THE OPTIMIZED COST FOR A DESIRED PRODUCTION RATE  $F_R \text{ kmol}/\text{hr}$ .

Total cost

$$C_T = C_M \cdot V + F_{AO} \cdot C_R \cdot \frac{Rs}{hr}$$

some depreciation cost is also added, not shown.

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

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

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

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

$\rightarrow F_R$  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 =  $\frac{C_T}{F_R} = \frac{V_{opt} C_M + F_{AO} C_R}{F_R}$

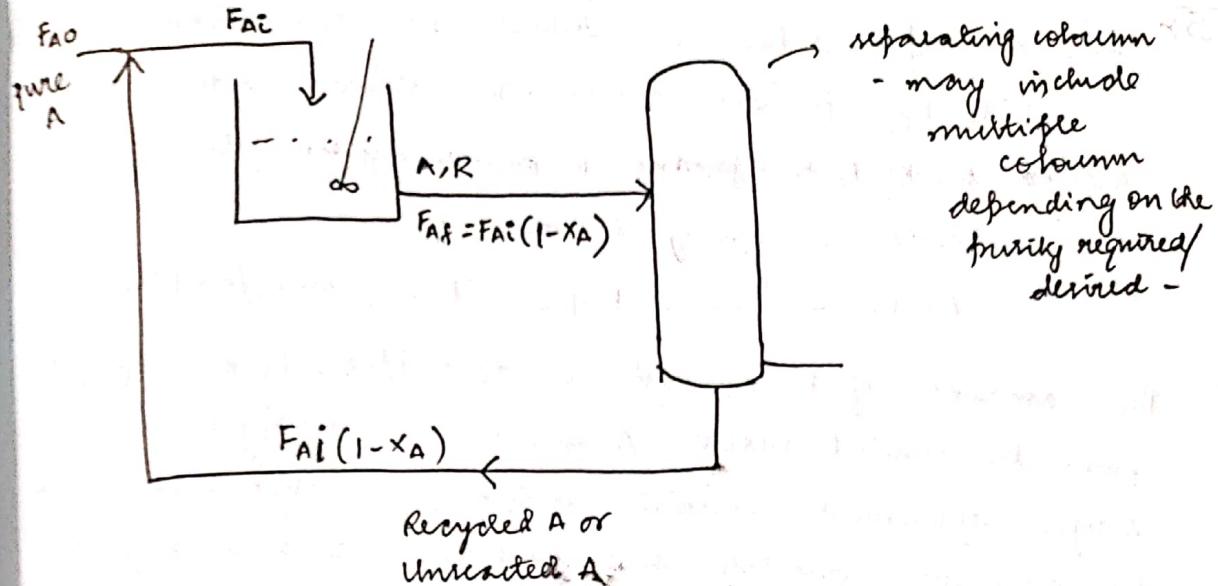
$$\left( \frac{Rs/hr}{kmol/hr} \right) = \frac{Rs}{kmol}$$

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.

$A \rightarrow R$



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

$C_S$  = unit cost of separation

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

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

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

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

Replacing  $F_{AI}$  with  $F_{AO}/x_A$ :

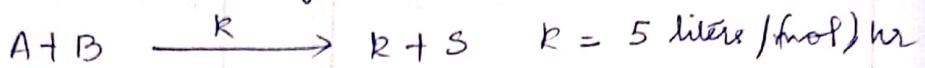
$$C_T = V_R C_M + F_{AO} \cdot C_R + \frac{F_{AO}}{x_A} (1-x_A) C_S$$

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

Find  $x_{A,opt}$

Problem

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 fed 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 & ₹ 0.18/hr/lit for mixed flow reactors.

Soln: Basis: 1 hr operation of CSTR



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

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

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

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

$$\frac{V}{V_0} = \frac{C_{A_0} X_A}{-r_A} = \frac{C_{B_0} X_B}{-r_B}$$

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

$$\Rightarrow F_{BO} = \frac{5 C_{AO} C_{BO} (1-x_A) (M-x_A) \cdot V}{x_A}$$

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

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

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

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

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

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

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

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

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

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

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

$$C_T = \frac{(56250.8 \times 0.205)}{10 \times 0.205 - 0.95} + \frac{6840}{10 \times 0.205 - 0.95}$$

$$= \frac{11115 + 6840}{1.13} = \frac{11531.25 + 6218.2}{1.13} = 17749.432$$

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

For PFR:

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

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

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

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

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

$$F_{BO} = F_{AO} \cdot \frac{C_{BO}}{C_{AO}} = 100 \cdot M$$

$$\Rightarrow \frac{dC_T}{dM} = 5625 + \frac{1360}{(M-1)^2} \left[ \frac{0.05M}{M-0.95} \left( \frac{M-1}{M^2} \right) \right] = 0 - \ln \left( \frac{M-0.95}{0.05M} \right)$$

$$\Rightarrow (M-1)^2 \times 5625 + 1360 \times 0.15 \frac{(M-1)}{M(M-0.95)} = 1360 \ln \frac{M-0.95}{0.05M}$$

By trial and error:  $M = 1.615$

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

$$\approx 5625 \text{ lit.}$$

putting the value of M:

$$C_T = 13746.85 \text{ \$}$$

$$V = \frac{2000}{0.615} \ln \frac{1.615 - 0.95}{(0.05)(1.615)} \\ = \underline{6856.56 \text{ liter}} \quad (\text{PFR when required})$$

- (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 :

$$C_{A0} = 0.6 \text{ moles/liter}$$

# (mole balance  
for 2 reactors)

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

# assume  $r_A = k C_A^n$

From reactor ①

$$\frac{V}{F_{A0}} = \frac{V}{V_0} C_{A0} = \frac{X_A}{K C_A^n} = \frac{C_{A0} - C_A}{C_{A0} \cdot K C_A^n}$$

empirical rate  
equation

$$\Rightarrow \frac{V}{V_0} = \frac{C_{A0} - C_A}{K C_A^n}$$

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

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

For second reaction  $v_0 = 50 \text{ cm}^3/\text{min}$

$$\frac{V}{v_0} = \frac{C_{A1} - C_{A2}}{KC_{A2}^n} = \frac{0.4}{0.05} = 8 \quad \textcircled{2} \quad \frac{C_{A2}}{C_{A0}} = \frac{0.6}{0.1}$$

$$\frac{V}{v_0} = 8 = \frac{C_{A0} - C_{A1}}{KC_{A1}^n} \quad \textcircled{3}$$

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

$$\textcircled{2} \rightarrow C_{A1} = (8 \times 0.0125) + 0.1 = 0.2$$

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

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

$$\textcircled{1} \textcircled{3} \quad \frac{K(0.1)^n}{K(0.2)^n} = 0.25$$

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

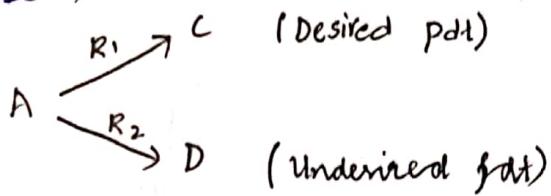
$$n = 2$$

$$K = 1.25$$

$$-r_A = 1.25 C_A^2$$

# Multiple Reactions

## - DESIGN OF PARALLEL REACTION -



For multiple reactions we need to consider 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, it is a good catalyst.

Consider:  $A + B \longrightarrow C \quad -r_{A1} = k_1 C_A C_B$

$A + B \longrightarrow D \quad -r_{A2} = k_2 C_A C_B$

50 mol A      30 mol of C

50 mol B      10 mol of D

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

$$\text{Selectivity of 'C'} = \frac{\text{Total moles of 'C' formed}}{\text{Total moles of 'D' formed}} \quad (\text{selectivity of C w.r.t. D})$$

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.

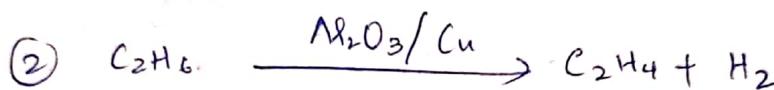
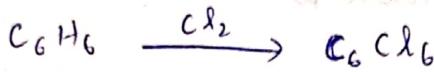
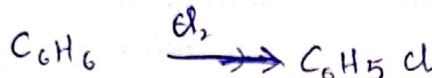
Under multiple reactions we have parallel and series.  
1<sup>st</sup> we will do the design of reactors in case of parallel reactions and we will 1<sup>st</sup> do the qualitative analysis.

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

reacted  
but not  
converted

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

EXAMPLE: ①



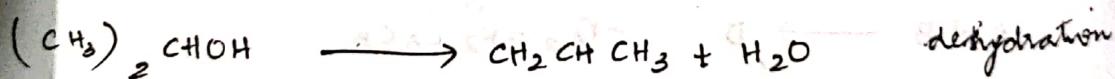
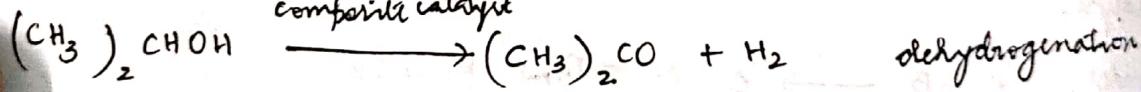
oxyacetylene flame;  $\text{C}_2\text{H}_4$  is one derived product

should be designed in such a way

that rate constant for 2nd reaction decreases

$\text{Cr}_2\text{O}_3, \text{TiO}_2$

composite catalyst



Dehydrogenation of Isopropanol  $\rightarrow$  acetone is produced.

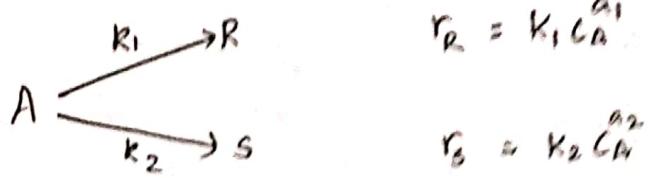
Deactivating product  $\rightarrow$  adsorbs on active sites, conversion

decreases  $\rightarrow$  Disadvantage of parallel reactions.

Transition metal or transition metal oxide in Alumina  
 $\downarrow$   
DEHYDROGENATION

heterogeneous  
catalysis

FCCMg  
Silica



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

CASE 1: If  $(a_1 - a_2) > 0$  (+ve) with  $A$  in concentration  $\uparrow$  velocity of  $R \uparrow$

CASE 2: If  $(a_1 - a_2) < 0$  (-ve) " " " "  $\downarrow$

CASE 3:  $(a_1 - a_2) = 0$  " " " independent of concentration

If 2 reactants are involved:

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

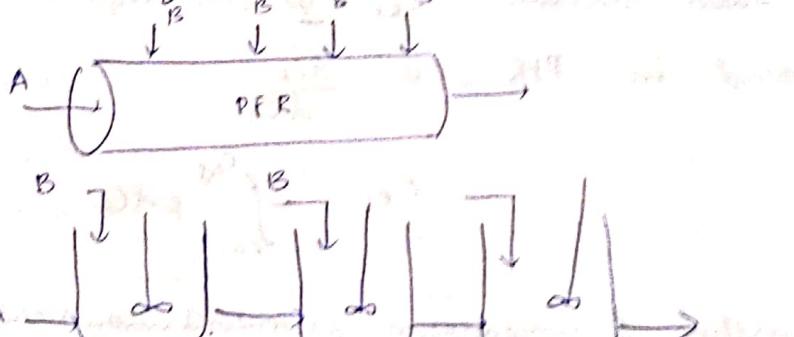


case (1): A, B both high

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 1: select desirable scheme



B to be kept low

A + main stream

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

## QUANTITATIVE DISCUSSION

Instantaneous yield :

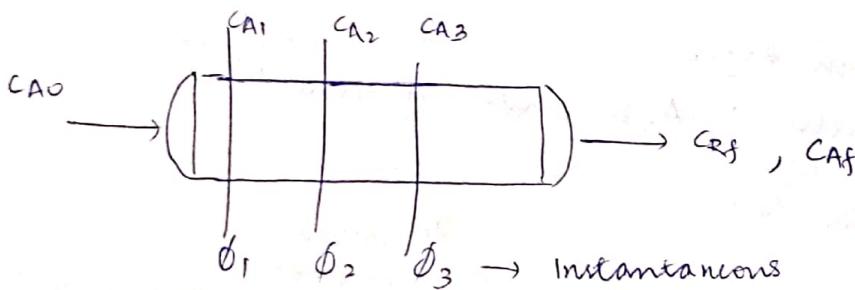
$$\phi = \frac{\text{moles of R formed}}{\text{moles of A reacted}} = \frac{dC_R}{-dC_A} = \text{instantaneous yield of R}$$

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

Overall yield :

$$\Phi = \frac{\text{all R formed}}{\text{all A reacted}} = \frac{C_{RF}}{C_{A0} - C_{Af}} = \frac{C_{RF}}{-\Delta C_A}$$

Exit concentration of R is  $C_{RF}$



In mixed reactor,  $C_{RF} = \Phi (C_{A0} - C_{Af})$

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

$$C_{RF} = - \int_{CA0}^{CAf} \phi dC_A$$

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

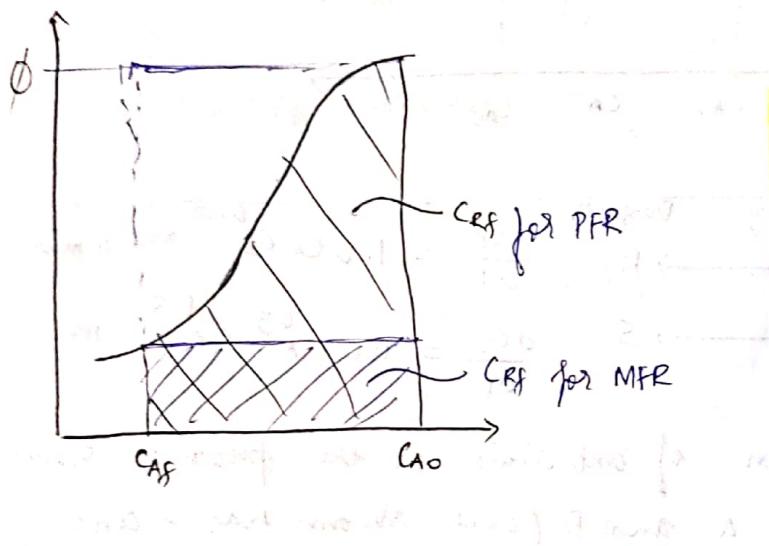
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In mixed reactor  $C_{RF} = \phi(C_{AO} - C_A)$

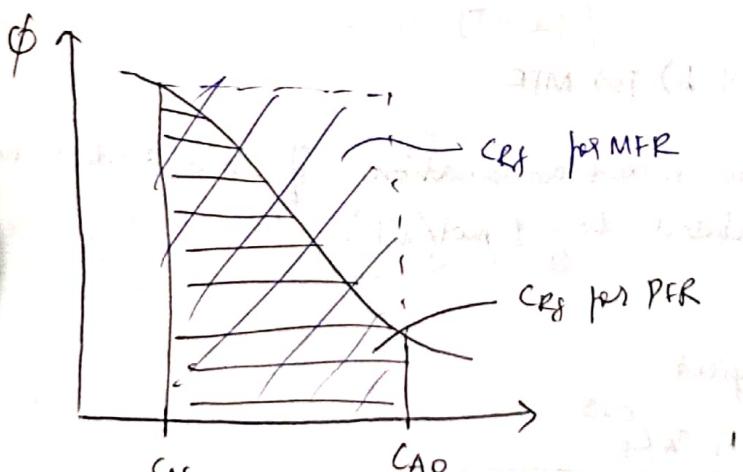
In PFR  $C_{RF} = - \int_{C_{AO}}^{C_A} \phi dC_A$

$$\phi = f(C_A)$$

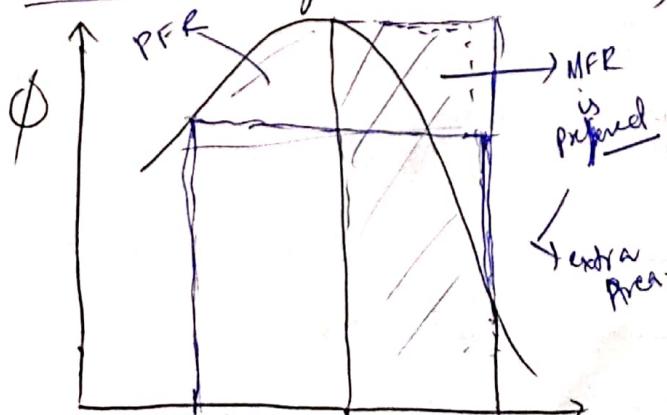
Example:  $\phi = \frac{1}{1+2C_A^2}$  or  $\phi = \frac{C_A^2}{C_A + 3C_A^2}$



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

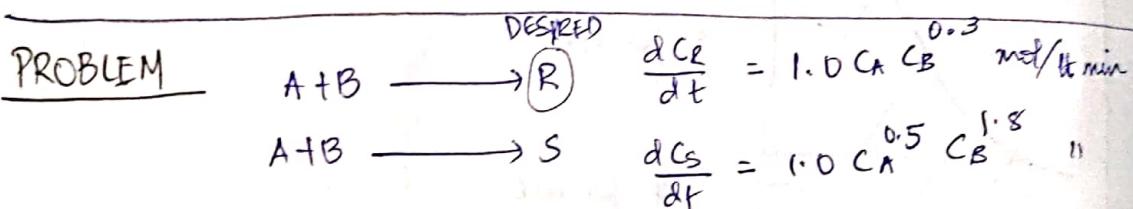
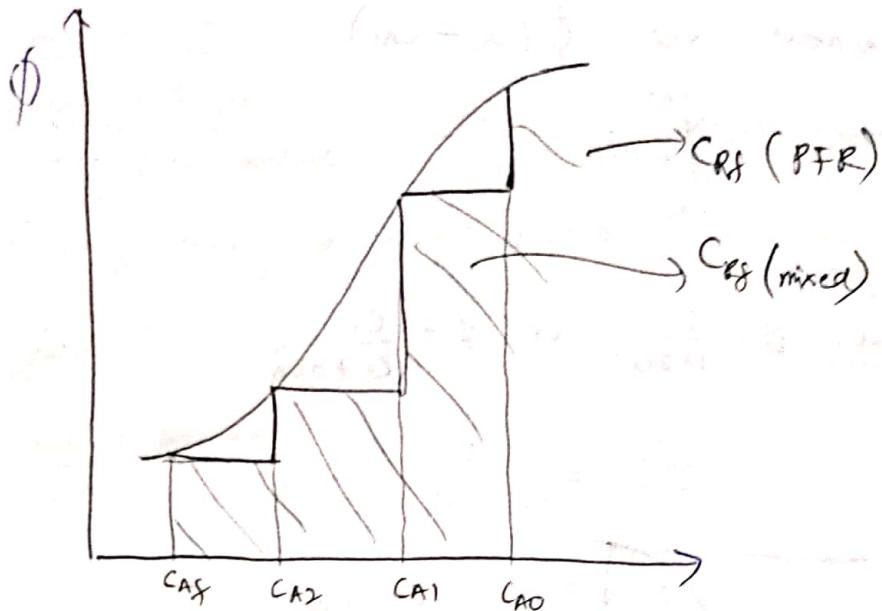


Autocatalytic reactions  $\rightarrow$



we have to optimize

Over time  
Relating to  
only the two  
equations



Find the fraction of impurities in the product stream for 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:

(i) with Instantaneous yield:

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

$$= \frac{1}{1 + C_A^{0.5} C_B^{1.8}}$$

(a) FOR PFR

$$A = 20 \text{ mol/lit}$$

$$B = 20 \text{ mol/lit}$$

$$C_{A0} = 10 \quad C_{AS} = 1$$

$$\Phi_p = \frac{C_{RF}}{C_{A0} - C_{AS}} = -\frac{1}{C_{A0} - C_{AS}} \int_{C_{A0}}^{C_{AS}} \phi dC_A.$$

$$= -\frac{1}{10-1} \int_{10}^1 \frac{1}{1 + \bar{C}_A^{0.5} C_B^{1.5}} dC_A$$

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

As  $C_A = C_B$  everywhere : —

$$\bar{\Phi}_p = -\frac{1}{10-1} \int_{10}^1 \frac{1}{1 + \bar{C}_A^{0.5} C_A^{1.5}} dC_A$$

$$= \frac{1}{9} \int_1^{10} \frac{dC_A}{1 + C_A}$$

$$= \frac{1}{9} \ln(1 + C_A) \Big|_1^{10}$$

$$\bar{\Phi}_p = 0.19$$

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

Concentration of Products : —

$$C_{RF} = (C_{A0} - C_{AS}) \bar{\Phi}_p$$

$$= (10-1) 0.19$$

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

$$C_{SF} = (C_{A0} - C_{AS})(1 - \bar{\Phi}_p)$$

$$= (10-1) 0.81$$

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

$$b) \text{ For MFR} \\ \phi = \frac{1}{1+C_{Af}} = \frac{1}{1+1} = \frac{1}{1+1} = 0.5$$

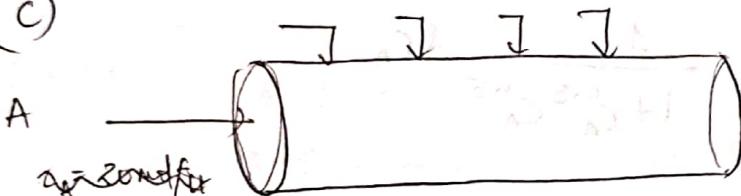
Inflow rate = 50%.

For MFR we evaluate  $\phi$  at exit:

$$\phi = \left. \frac{1}{1+C_A} \right|_{exit} \approx \frac{1}{1+C_{Af}}$$

~~Extrusion fraction is function of position of exit~~

(c)



$$C_{B_0} = 1 \text{ mol/lit.} \quad C_{Af} = 1$$

$$C_{A_0} = 19 \text{ mol/lit.}$$

$$\phi = \frac{1}{C_{A_0} - C_{Af}} \int_{18}^1 \frac{dC_A}{1 + C_A^{-0.5}} \quad C_B = 1$$

$$= \frac{1}{18} \int_1^{19} \frac{dC_A}{1 + C_A^{-0.5}} = \frac{1}{18} \left[ (19-1) - 2(\sqrt{19}-1) + 2 \ln \frac{1+\sqrt{19}}{2} \right] \\ = 0.741$$

(Question — maximum yield  $\rightarrow$  find optimum  $\phi$ )  
 $A \xrightarrow{R} R_1 C_A = r_R$   
 $A \xrightarrow{S} R_2 C_A = r_S$   
 $A \xrightarrow{T} R_3 C_A = r_T$   $\rightarrow$  Overall product. fraction desired  $\phi$ .

$$\phi = \frac{r_S}{r_R + r_S + r_T} = f(C_A) = f(C_A)$$

$$\frac{d\phi}{dC_A} = f'(C_A) = 0$$

$$\phi_{opt} = ?$$

$C_{sf,max} = ?$

write expression for  $C_{sf}$

$$\frac{dC_{sf}}{dC_A}$$

$\rightarrow C_{smax}$

Find MFR

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

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

We will  $C_{A,off}$  from this expression.

↓

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

IT is difficult to calculate  $\phi$  for

ratio of different variables

so we calculate  $\phi$  with

constant values

and then do

it again

Effect of  $A$  &  $K$

on  $\phi$

so

so

so

so

so

so

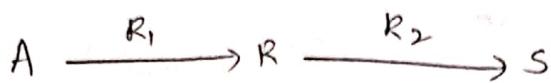
so

so

so

# SERIES MULTIPLE REACTIONS

(Qualitative Analysis)



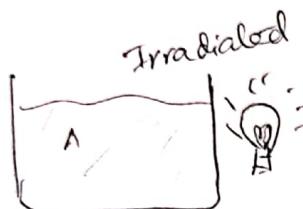
Series reaction  
1st order

$R_1, R_2$  rate constants ( $t_{1/2}$ )

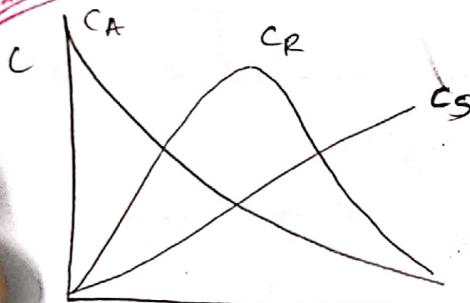
$$-r_A = R_1 C_A$$

$$+r_R = R_1 C_A - R_2 C_R$$

$$r_S = R_2 C_R$$



1st CASE



As R forms, A & R will fight for light

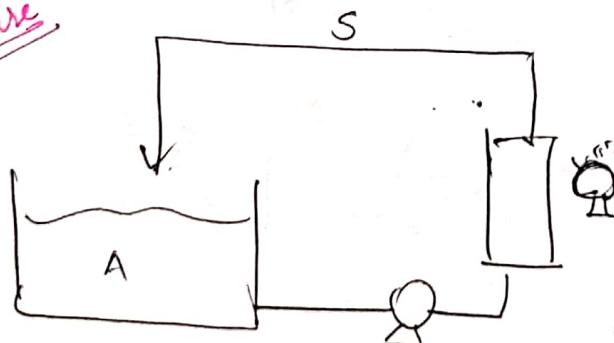
It is similar to Batch reactor & PFR.

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

Behaviors of Batch & PFR

$\rightarrow$  R is Desired product.

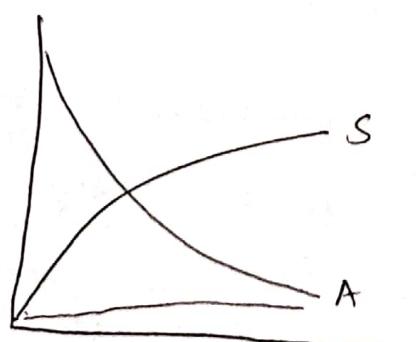
2nd case



Our product will be 'S'

R will be in traces.

'S' AS DESIRED PRODUCT

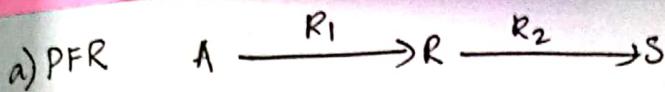


(THEORY + PROB Imp in this chapter)

# Quantitative Analysis

## Series

17/10/19



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

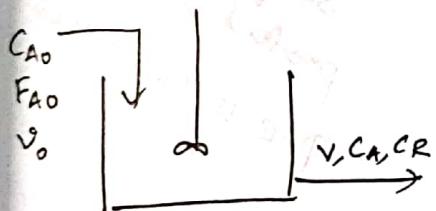
$$\frac{C_A}{C_{A_0}} = e^{-k_1 z}$$

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

$$z_{D,opt} = \frac{1}{K_2 - k_1}$$

$$z_{D,opt} = \frac{\ln \left( \frac{k_2}{k_1} \right)}{k_2 - k_1} \quad (1)$$

b) MFR



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

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

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

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

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

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

A balance

$$v C_{A_0} = v C_A + k_1 C_A V$$

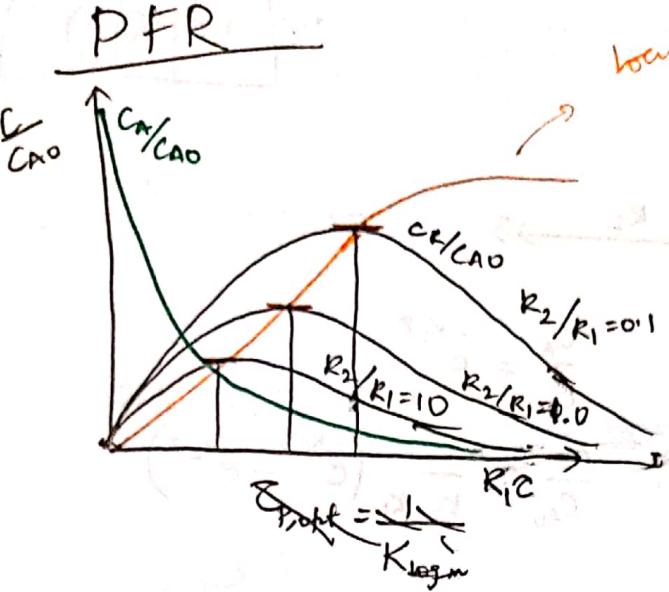
$$\frac{C_A}{C_{A_0}} = \frac{1}{1 + k_1 z_m}$$

R-balance

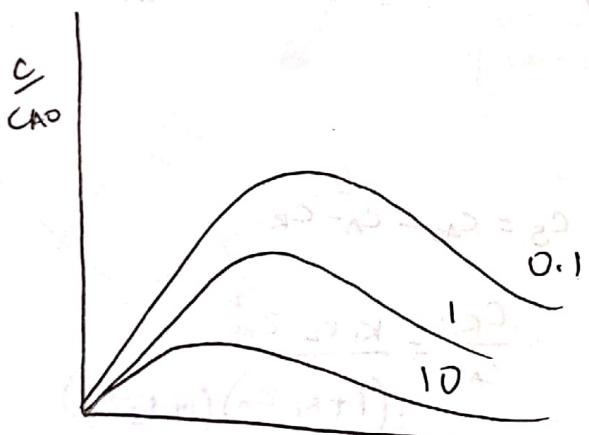
$$v C_{R_0} = v C_R + (-r_R) V$$

$$0 = v C_R + (-k_1 C_A + k_2 C_R) V$$

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



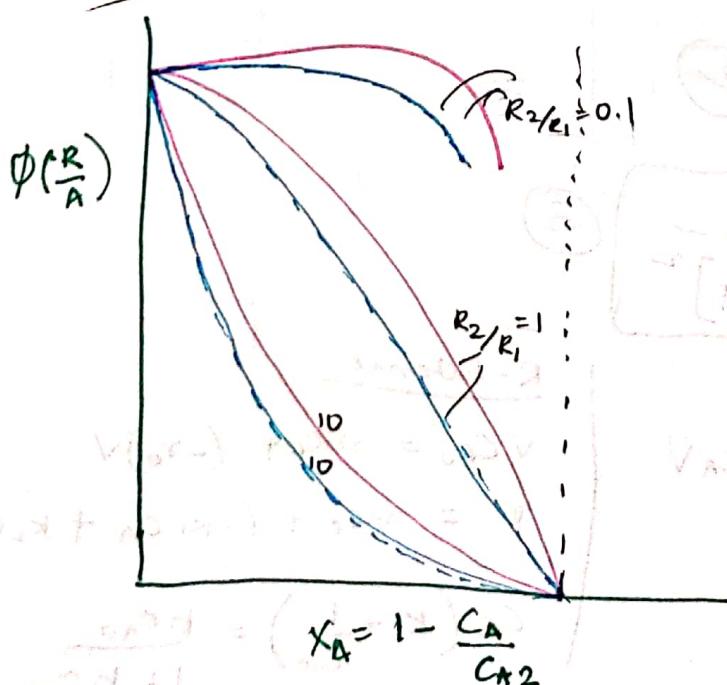
MFR



10/10/19

instantaneous yield vs conversion

PFR  
MFR



Theoretical questions related to Design - When we will choose which?

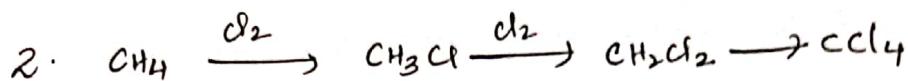
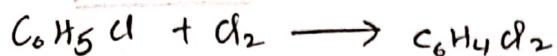
of the plots for CSTR & PFR are plotted together MFR will always be lower than PFR So if our desired product is  $R^*$ , then PFR is PREFERRED!

if  $R_2/R_1$  is large low conversion levels are chosen to get high  $\phi$

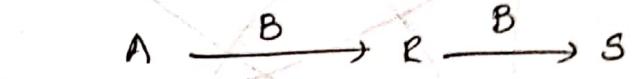
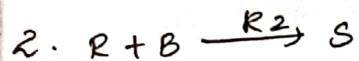
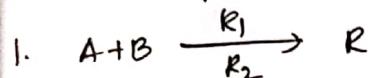
↓ conversion is low ∵ large reactor required

more well?

# — SERIES PARALLEL COMBINATION —



General form



$$\frac{dC_A}{dt} = -k_1 C_A C_B$$

$$\frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_R C_B$$

$$\frac{dC_S}{dt} = k_2 C_R C_B = \frac{dC_S}{dt}$$

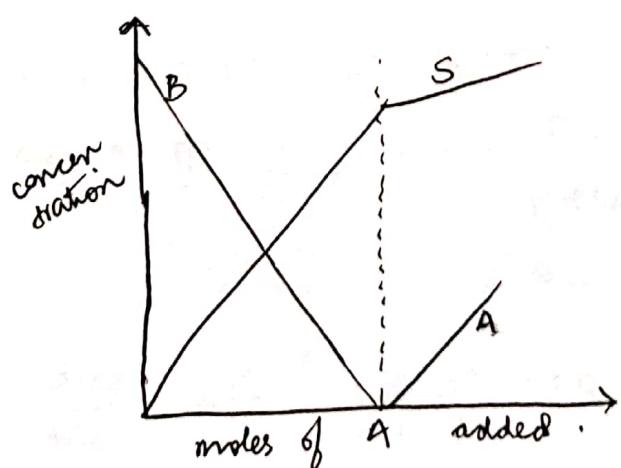
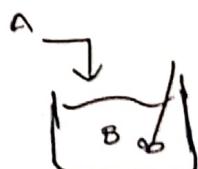
$$\frac{dC_R}{dt} = k_1 C_A C_B - k_2 C_R C_B$$

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.

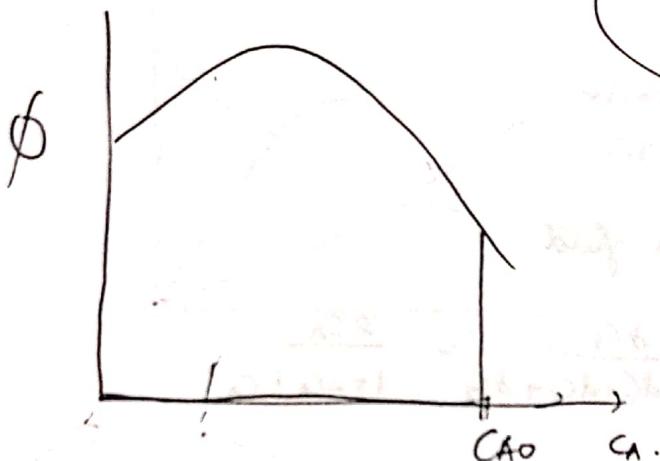


(no R → because small amount of A is added to excess B)

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

$$C_{St, \max} = \left. \frac{2 C_A}{(1+C_A)^2} (C_{A0} - C_A) \right|_{C_A=0.5} = 0.666$$

PFR



We have to see  
when we get  
maximum  
when  
 $C_A = 0$ .

$$C_{St, \max} = - \int_0^0 \phi dC_A.$$

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

$$= 2 \left[ \ln x - \frac{1}{x} \right]_0^2$$

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

$$= 0.864.$$

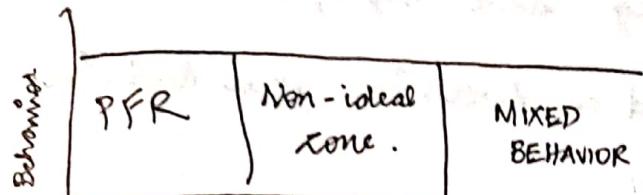
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# - NON-IDEAL REACTORS -

Ideal Behavior:

(1) No axial mixing (PFR)

(2) Complete mixing (ideal CSTR)



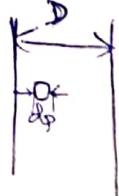
Extent of mixing

What are causes of Non-ideal Behavior?

Derivation from ideal behavior are due to following reasons:

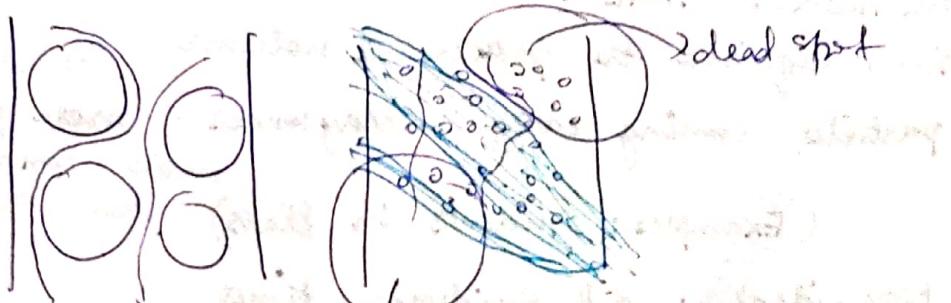
- (1) Element of fluid may move at different velocities causing channeling.
- (2) Creation of stagnant point or dead spots or partially aggregated segregated as they move.
- (3) The extent of micromixing, diffusion in the direction of flow or dispersion.

(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.

$\begin{array}{c} \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \end{array}$	JM Smith Dispersion micromixing	dispersion coefficient $D_e$ dispersion number $\frac{D_e}{UL}$ (similar to pelet no)
---	---------------------------------------	---

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

\* Four methods are used to determine stir deviation.

#### (CELL BALANCE METHOD)

1. Segregated flow model

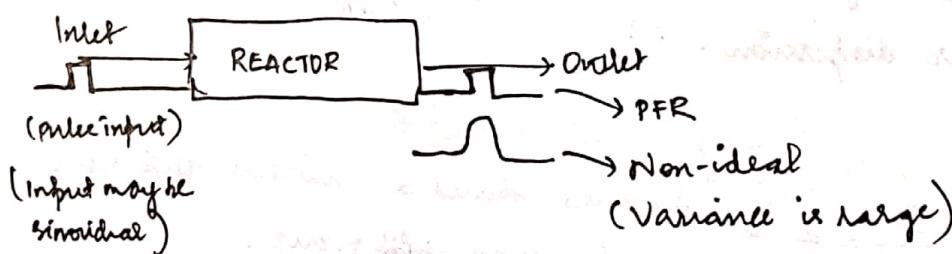
2. Dispersion model

3. CSTR in series model

4. Recycle Reactor model

} theoretical model.

EXPERIMENTALLY  $\rightarrow$  RTD method  $\rightarrow$  residence time distribution tracer technique (tracer - inert).

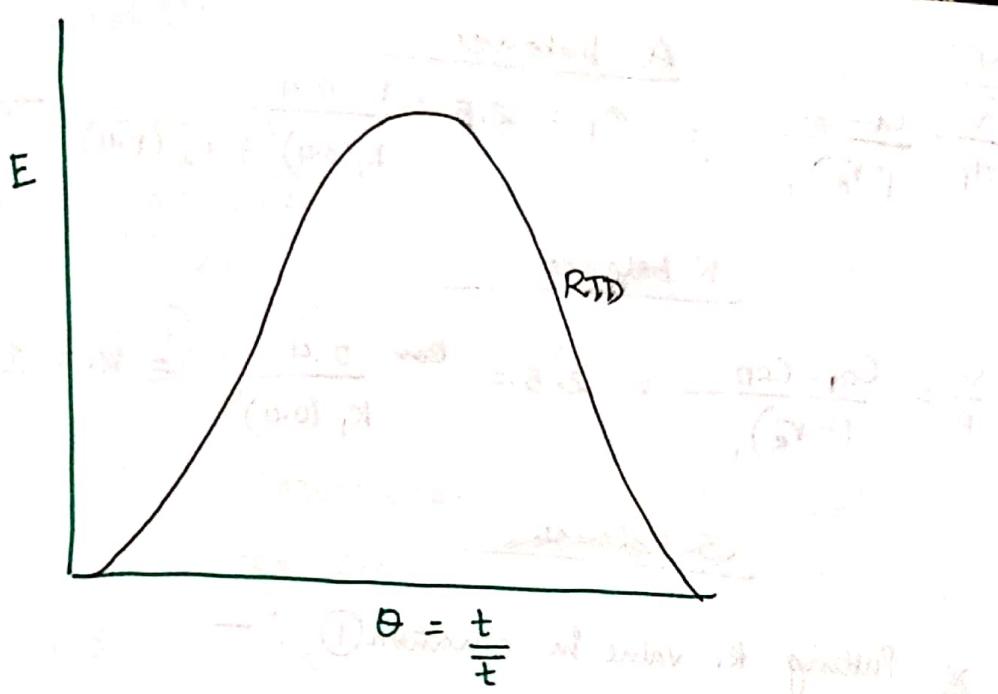


#### RESIDENCE TIME :

Time required to process 1 volume particles coming early - stay longer - more reaction -  
 (Examples: Students in class) .

Non-ideal - diff Residence times

Ideal - Same residence time.

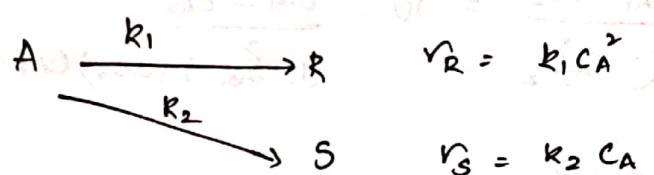


$\bar{t}$  = Average residence time

$\theta$  = 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 ( $\tau_1 = 2.5 \text{ min}$

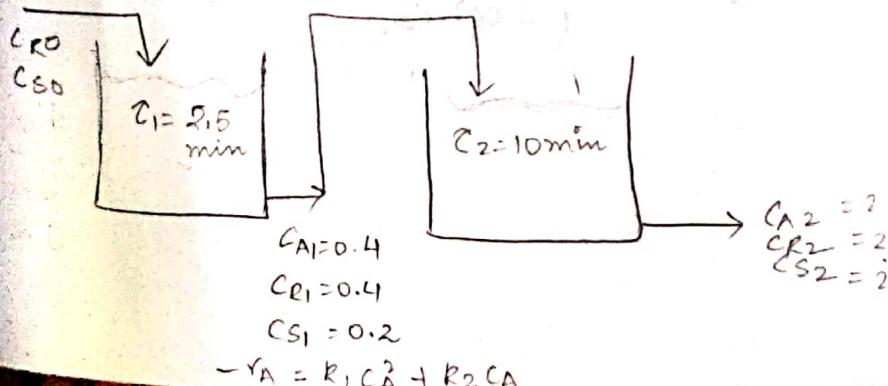
$\tau_2 = 10 \text{ min}$ ).  $C_{A1} = 0.4 \text{ mole/l}$

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

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

Find the composition leaving second reactor.

$$C_{A0} = 1$$



CSTR 1

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

A balance

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

S balance

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

$$R_2 = \frac{1 - 0.4}{2.5} - R_1(0.4)^2 \quad 0.4 \cdot R_1 + R_2 = 0.6 \\ = 0.08 \text{ min}^{-1} \quad R_2 = 0.6 - 0.4 = 0.2$$

CSTR 2

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

R balance

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

S balance

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

From equation ① :

$$10C_{A_2}^2 + 3CA_2 - 0.4 = 0$$

$$CA_2 = \frac{-3 \pm \sqrt{9+16}}{20}$$

$$= 0.1, -0.4$$

$$CA_2 = 0.1$$

From eq ② :  $CR_2 = 1.0$

$$CR_2 = 0.5$$

$$CR_2 = 0.5$$

$$CS_2 = 0.4$$

From eq ③  $CS_2 =$

A and B react with each other as follows



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

$$2A \rightarrow R$$

$$A+B \rightarrow S$$

$$2B \rightarrow T$$

Now find the molarities of A and B

(A.M.C)

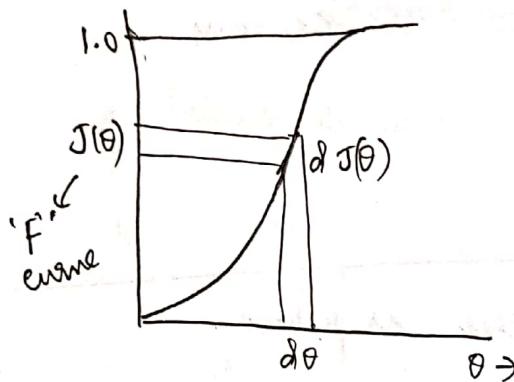
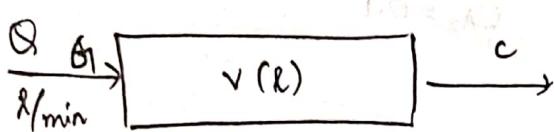
for A and B

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## - RESIDENCE TIME DISTRIBUTION -

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

At  $\theta = 0$ ,  $J(\theta) = 0$ .



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

$$\bar{\theta} = \frac{\int_0^1 \theta d J(\theta)}{\int_0^1 d J(\theta)} = \int_0^1 \theta d J(\theta) = \frac{V}{Q} \text{ or } \frac{V}{Q} \rightarrow \text{for Ideal Reactor}$$

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

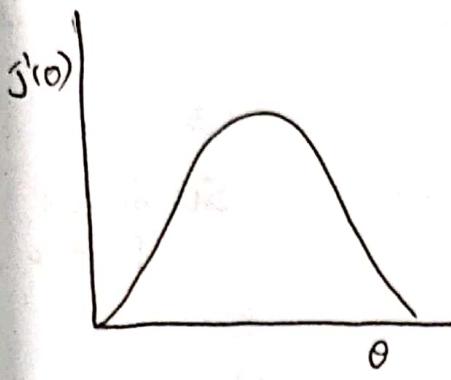
$$d J(\theta) = J'(\theta) d\theta$$

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

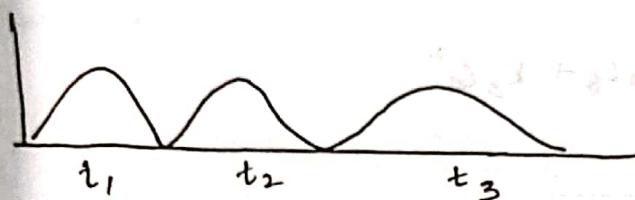
E curve is the plot of E vs  $\theta$  or t (J.M. Smith)  
follows

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

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



Distribution curve



Variation of RTD  
Flow behavior  
- Conversion will change

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

$$= \int_0^\infty \theta J'(\theta) d\theta$$

(Generalized \$ see)

Discrete method

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

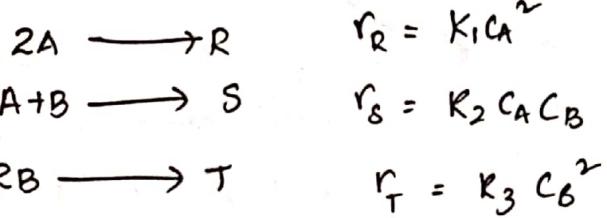
$$\bar{t} = \sum t E \Delta t$$

t	E	txE	tEΔt
0	1	0	0
15	1	15	15
20	1	20	20
25	1	25	25
30	1	30	30
35	1	35	35

$\Delta t$  ↓  
Interval has to be equal

TUTORIAL

①

Sis desired  
product.

$$\text{Let } z = \frac{c_A}{c_B}$$

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

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

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

$$\frac{d\phi}{dz} = 0$$

$$(k_1 z^2 + k_2 z + k_3) k_2 - k_2 z (2k_1 z + k_2) = 0.$$

$$k_1 k_2 z^2 + k_1 k_2 z + k_1 k_2 k_3 z^2 - 2k_2 k_1 z^2 - k_2^2 z = 0.$$

$$k_1 k_2 z^2 = k_2 k_3$$

$$z^2 = \frac{k_2 k_3}{k_1 k_2} = \frac{k_3}{k_1}$$

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

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

Assignment 3

Prob 5



Given:

$$\frac{C_{AO}}{C_{BO}} = 9$$

$$\frac{C_A}{C_B} = 100 \text{ (initial)}$$

how much D = ?

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

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

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

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

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

$$\frac{100 C_{Bf}}{C_{AO}} = \frac{(C_{Bf})^{1/7}}{(C_{BO})^{1/7}}$$

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

$$C_{Bf} = 0.358$$

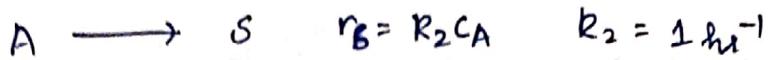
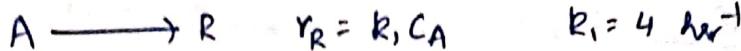
$$C_{Bf} = 0.301 \text{ mol/lit.}$$

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

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

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

Prob 8



Given:

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

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

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

Unconverted A is not recycled.

SOP: Basis = 1 hour operation

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

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

CSTR

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

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

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

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

$$C_{A0} = 1$$

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

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

$$\frac{1 - x_A + x_A}{x_A} = \frac{F_{AO} + 100}{100}$$

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

$$P = P_{\text{profit}} = 5F_R - 25 - 2.25 F_{AO}$$

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

$$= \frac{4 F_{AO} 100}{100 + F_{AO}} - 25 - 2.25 F_{AO}$$

$$\frac{\partial P}{\partial F_{AO}} = 0 = \frac{400 (F_{AO} + 100) - F_{AO} \cdot 1}{(F_{AO} + 100)^2} - 0 - 2.25 = 0$$

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

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

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

$$F_{AO} = 33.33$$

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

3/10/19 ~ RTD FOR KNOWN MIXING CONDITIONS

Example : CSTR

Tracer : Step input function

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

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

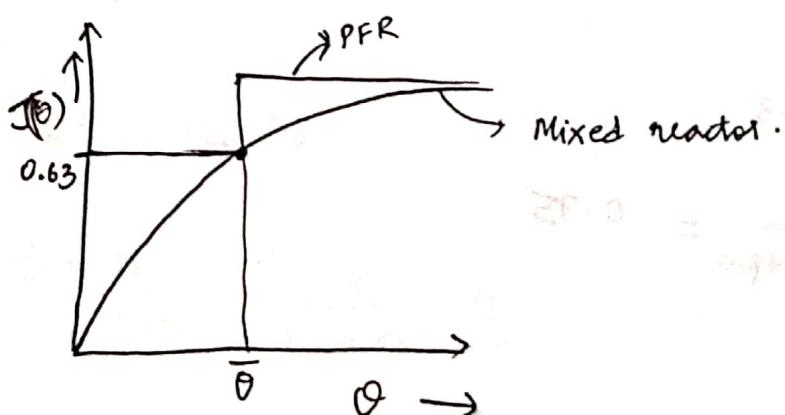
for  $\Delta \theta$  time, concentration change:  $\Delta C$ .

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

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

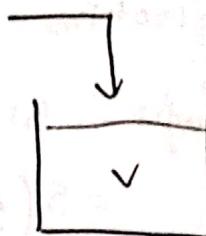
$$\Rightarrow -\ln \left[ \frac{C_0 - c}{C_0} \right] = \frac{\theta}{\Theta}$$

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



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

$C_0, Q$



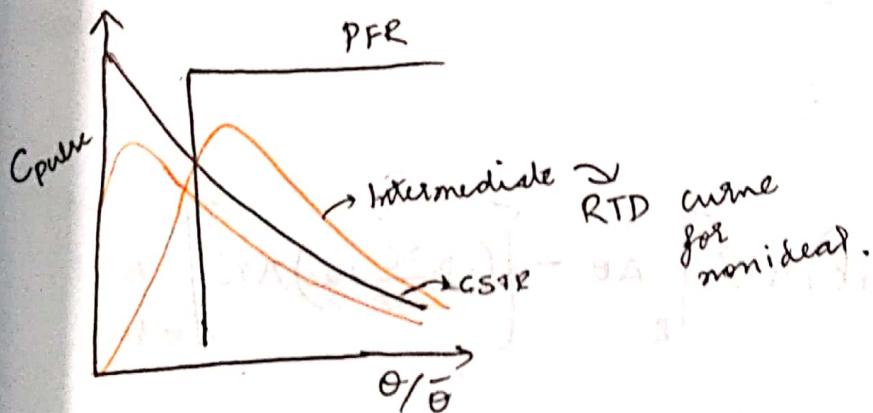
$$J'(\theta) = \frac{1}{\theta} e^{-\theta/\theta}$$

Again we have :

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

$$= C_0 \Delta t_0 \frac{1}{\theta} e^{-\theta/\theta}$$

JM  
Smith



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

$$E_{curve} = \frac{C_{pulse}}{\int_0^{\infty} C_{pulse} d\theta} = \frac{C_0 \Delta t_0 \frac{1}{\theta} e^{-\theta/\theta}}{\int_0^{\infty} C_0 \Delta t_0 \frac{1}{\theta} e^{-\theta/\theta} d\theta}$$

$$= \frac{C_0 \Delta t_0}{\int_0^{\infty} \frac{1}{\theta} e^{-\theta/\theta} d\theta}$$

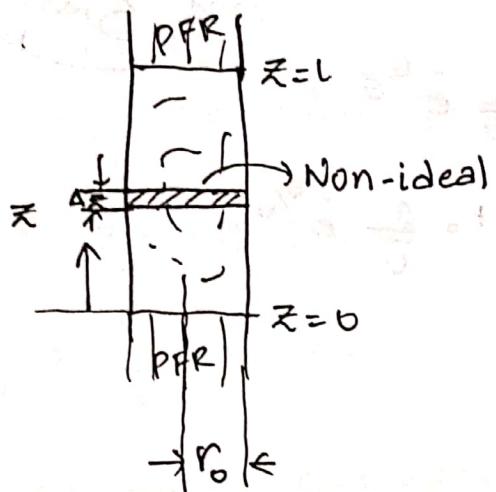
Integrating factor is  $\theta^{1/\theta}$

$\int_0^{\infty} \theta^{1/\theta} d\theta = \Gamma(1 + 1/\theta)$

Integration factor is  $\theta^{1/\theta}$

Factor is  $\theta^{1/\theta}$

# 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  $z=0$ , set 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 need to describe initial  
the reactor

②  $z=L, \theta \geq 0$

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

(With these conditions,  
not possible to solve)

Transforming variables to DIMENSIONLESS:

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

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

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

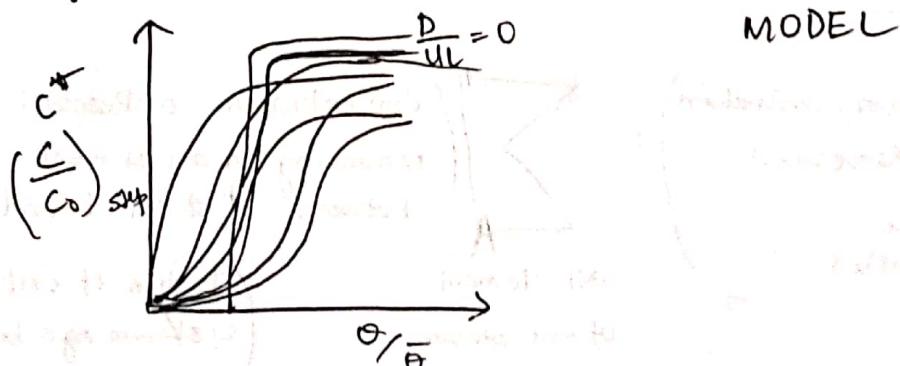
From this we get :

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

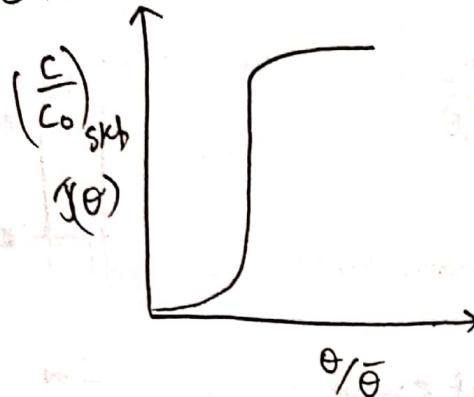
$$C^*_{z=L} = \left( \frac{C}{C_0} \right)_{\text{step}} = \frac{1}{2} \left[ e^{-1 - \operatorname{erf} \left( \frac{1}{2} \sqrt{UL} \frac{1 - \theta/\bar{\theta}}{\sqrt{\theta/\bar{\theta}}} \right)} \right]$$

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

Varying the dispersion number, we will get series of curve of  $C^*$  vs  $\theta/\bar{\theta}$  → DISPERSION MODEL



# DISPERSION MODEL



If the plot is like this,  
it is close to PFR,

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

$0.1, 0.2 \rightarrow$  Non ideal types.

$0.001 \rightarrow$  very close

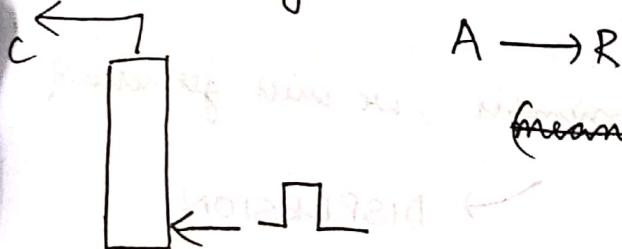
we can  
directly use  
PFR equation

Unknown reactor

RTD plot, 2  
for particular  $\frac{D_L}{UL}$  value,  
Extraction  $\rightarrow$  conversion from  $\frac{D_L}{UL}$

## CONVERSION FROM RTD:-

- RTD is already determined.



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

(fraction of exit stream  
of stream age between  
and  $t + \Delta t$ )

Concentration of Reactant  
remaining in an element  
between  $t$  and  $t + \Delta t$

(fraction of exit stream  
of stream age between  
and  $t + \Delta t$ )

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

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:

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

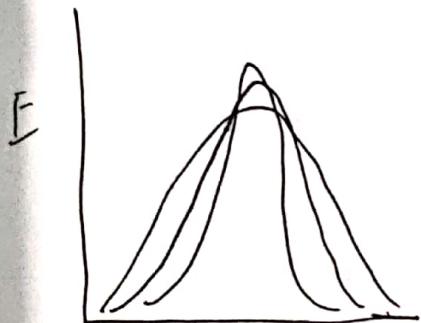
$$\bar{C}_A = C_{A0} \int_0^{\infty} e^{-kt} E dt$$

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

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

From average concentration we can find average conversion.

For different Enymes, calculate Variance.



$$\text{Variance} = \sigma^2$$

$$= \int_0^{\infty} (t - \bar{t})^2 C dt$$

$\int_0^{\infty} C dt$

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

We can use this summation method if -  
 • 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 concentrations measured at the exit.

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

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

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

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

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

Steps :-

- ① E curve
- ② average 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 -