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Department: Chemical Engineering

Subject: Chemical Reaction Engineering

Unit: III

Topic: Reactors in Series

LECTURE :- SIZE COMPARISIONS OF SINGLE AND MULTIPLE REACTORS

⁕) OUTLINE :- 1) INTRODUCTION
2) SIZE COMPARISION OF SINGLE REACTORS
3) SIZE COMPARISION OF MULTIPLE REACTORS

1) Fluids can be processed by i) Single batch and flow reactors ii) Series of reactors, and iii) recycle of product stream.

⇒ BATCH REACTORS :-
- Advantages :- 1) Small instrumentation cost
2) flexibility of operation
- Disadvantages :- 1) High labour and handling cost
2) High shutdown times between batches.

→ To calculate reactor sizes for constant density $\boxed{\varepsilon = 0}$ and for a given duty - Same volume is required. However, PFR is advantageous due to above reasons.

⇒ SIZE COMPARISION BETWEEN PFR ~~AND~~ MFR
→ For 1st and 2nd order reactions :-
★ For a given duty the ratio of sizes of MFR and PFR depends on
1) Extent of reaction 2) Stoichiometry 3) Form of rate eq.

→ Considering general rate equation :-
For n^{th} order :- $\boxed{-r_A = -\frac{1}{V}\frac{dN_A}{dt} = kC_A^n}$ 'n' varies from 0 to 3.

For MFR :- $\tau_m = \left(\frac{C_{A0}V}{F_{A0}}\right)_M = \frac{C_{A0}X_A}{-r_A}$

$\therefore$ For n^{th} order :- $\tau_m = \frac{1}{kC_{A0}^{n-1}}\frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}$ —①

For PFR :- $\tau_p = \left(\frac{C_{A0}V}{F_{A0}}\right)_P = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A}$

For n^{th} order :- $\tau_p = \frac{1}{kC_{A0}^{n-1}}\int_0^{X_A}\frac{(1+\varepsilon_A X_A)^n}{(1-X_A)^n}dX_A$ —②

Divide ① by ②

$$\frac{(\tau C_{A0}^{n-1})_M}{(\tau C_{A0}^{n-1})_P} = \frac{\left(\frac{C_{A0}^n.V}{F_{A0}}\right)_M}{\left(\frac{C_{A0}^n.V}{F_{A0}}\right)_P} = \frac{\left[X_A\left(\frac{1+\varepsilon_A X_A}{1-X_A}\right)^n\right]_M}{\left[\int_0^{X_A}\left(\frac{1+\varepsilon_A X_A}{1-X_A}\right)^n dX_A\right]_P}$$

—③

⇒ For constant density system ; $\varepsilon_A = 0$

the expression can be integrated to obtain

$$\frac{(\tau C_{A0}^{n-1})_M}{(\tau C_{A0}^{n-1})_P} = \frac{\left[\frac{X_A}{(1-X_A)^n}\right]_M}{\left[\frac{(1-X_A)^{1-n}-1}{n-1}\right]_P} \quad ; \text{ for } n \neq 1$$

For $n = 1$

$$\frac{(\tau C_{A0}^{n-1})_M}{(\tau C_{A0}^{n-1})_P} = \frac{\left(\frac{X_A}{1-X_A}\right)_M}{[-\ln(1-X_A)]_P} \quad \text{---} \quad (4)$$

⇒ For 2nd order

→ Variation of reactant ratio :

$$A + B \longrightarrow P \quad ; \quad -r_A = -r_B = k C_A C_B \quad ; \quad M = \frac{C_{B0}}{C_{A0}}$$

For $M = 1$; $C_{B0} = C_{A0}$

The reaction becomes

$$2A \longrightarrow P \quad ; \quad -r_A = k C_A^2$$

→ If one reactant is in excess $[C_B \approx C_{B0}]$

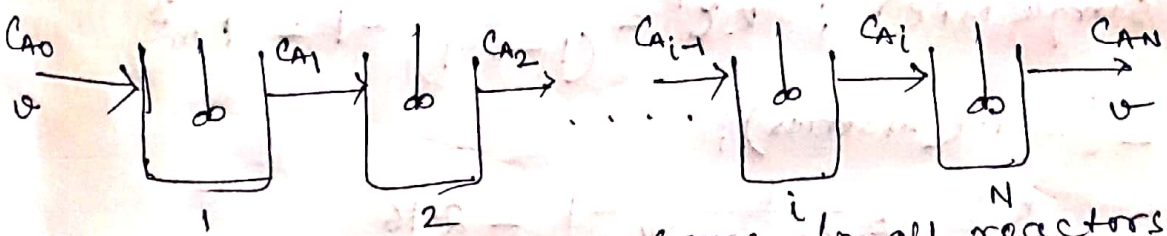
$$-r_A = k C_A C_B = (k C_{B0}) C_A = k' C_A \quad \text{where } k' = k C_{B0}$$

→ behaves as pseudo 1st order reaction [when $M \gg 1$]

NOTE :- A simple observation of design equation of MFR and PFR will show that the volume of MFR is always larger than that of PFR for a given conversion X_A. [REFER LEVENSPIEL PLOT]

⇒ REACTOR DESIGN AND COMBINATION OF REACTORS :-

→ let us assume MFR's in series for a 1st order steady state reaction. [Liquid phase reaction → as MFRs are used only for liquid phase rxn]



Assume volumes are same for all reactors

$\therefore V_1 = V_2 = V_i = V_N = V$

Again let τ_i constant ; $\tau_i = \frac{V_i}{v}$ [τ_i is space time]

refer definition of τ_i

∴ Total time $\tau = N\tau_i = \frac{NV_i}{\upsilon} = \frac{V'}{\upsilon}$ [where $V' = \sum_i^N V_i$]

⇒ We have to determine $\frac{C_{AN}}{C_{A0}} \left[= (1 - X_{AN})\right]$ [$\because C_{Ai} = C_{A0}(1 - X_A)$]

⇒ Material balance over each reactor;—

Reactor (1) ⇒ $\upsilon C_{A0} = \upsilon C_{A1} + (kC_{A1})V$ ——(1)

$\therefore \frac{C_{A1}}{C_{A0}} = \frac{1}{1+k\tau}$ ——(2) $\left[\tau = \frac{V}{\upsilon}\right]$

for (2) ⇒ $\upsilon C_{A1} = \upsilon C_{A2} + (kC_{A2})V$ ——(3)

$\therefore \frac{C_{A2}}{C_{A1}} = \frac{1}{1+k\tau}$

(3) ⇒ $\frac{C_{A3}}{C_{A2}} = \frac{1}{1+k\tau}$ ——[follow above method]

for (N) ⇒ $\frac{C_{AN}}{C_{AN-1}} = \frac{1}{1+k\tau}$

∴ Multiplying all terms :—

$\frac{C_{A1}}{C_{A0}} \cdot \frac{C_{A2}}{C_{A1}} \cdots \frac{C_{AN-1}}{C_{AN-2}} \cdot \frac{C_{AN}}{C_{AN-1}} = \frac{C_{AN}}{C_{A0}} = \frac{1}{(1+k\tau)^N}$ ——(5)

$\therefore \frac{1}{\left[1 + \left(k\frac{\tau'}{N}\right)^N\right]} = (1 - X_{AN})$

$\therefore \frac{k\tau'}{N} = (1 - X_A)^{-1/N} - 1$ ——(6)

⇒ considering $N = 1$; eq. (5) becomes $k\tau' = \left(\frac{1}{1-X_A}\right) - 1$

or $k\tau' = \left(\frac{X_A}{1-X_A}\right)$ → Refer Damköhler No. lecture.

⇒ Let us assume $X_A = 0.9$

$N = 1$ (single MFR) ; $k\tau' = \frac{1}{(1-0.9)} - 1 = 9\ m^3$

for $N = 2$ (2 MFR in series);

$\frac{k\tau'}{2} = \frac{1}{(1-0.9)^{1/2}} - 1 = 2.16$

$\therefore k\tau' = 4.325\ m^3$

Signifies a combined vol. of $4.325\ m^3$ consisting of 2 MFRs of $2.16\ m^3$ volume of each.

Calculate for $N = 3$; $(k\tau' = 3.413\ m^3)$; $N = 4$ $(k\tau' = 3.113\ m^3)$

Let us consider $N = \infty$

$$k\tau' = -\ln(1 - X_A) = 2.302\ m^3$$ [Refers to a PFR (refer to eq. (4))]

⇒ SIGNIFICANCE OF THE LECTURE :—

1) At constant density, for a given conversion $(X_A = 0.9)$ a single MFR requires larger volume as compared to a series of MFRs.

2) There is constant mixing of new reactants, however it does not mean there is constant reaction. Hence the product contains both reacted and unreacted molecules. This is the reason why a single MFR requires larger volume.

3) In case of PFR, a batch of molecules spend the same time within the reactor. Hence a smaller volume is required.

———— x ———— x ————

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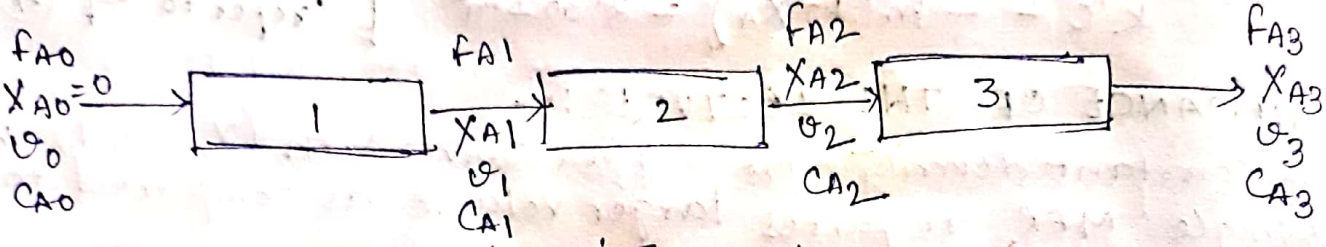
LECTURE: PFR AND MFR IN SERIES

=> Let us first assume 3 PFRs in series :—



for constant density system

$$v_0 = v_1 = v_2 = v_3 = v$$

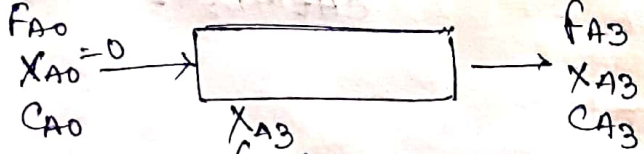
Material balance :—

$$F_{A0}\, dX_A = -r_A\, dV \quad \longrightarrow (1)$$

Again $$\frac{V}{F_{A0}} = \sum \frac{V_i}{F_{A0}} = \frac{V_1}{F_{A0}} + \frac{V_2}{F_{A0}} + \frac{V_3}{F_{A0}} \quad \longrightarrow (2)$$

$$\therefore \frac{V}{F_{A0}} = \int_0^{X_{A1}} \frac{dX_A}{-r_A} + \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{-r_A} + \int_{X_{A2}}^{X_{A3}} \frac{dX_A}{-r_A} \quad \longrightarrow (3)$$

Again if there is a single reactor ; we have



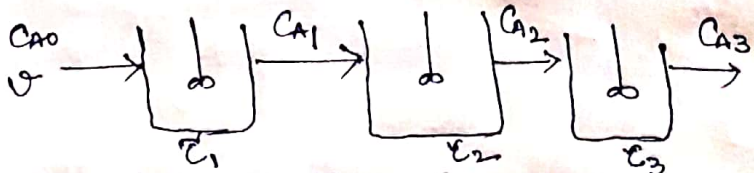
$$\therefore \frac{V}{F_{A0}} = \int_0^{X_{A3}} \frac{dX_A}{-r_A} \quad \longrightarrow (4)$$

Equation (4) can be split algebraically

$$\frac{V}{F_{A0}} = \int_0^{X_{A1}} \frac{dX_A}{-r_A} + \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{-r_A} + \int_{X_{A2}}^{X_{A3}} \frac{dX_A}{-r_A} \quad \longrightarrow (5)$$

which is similar to equation (3)

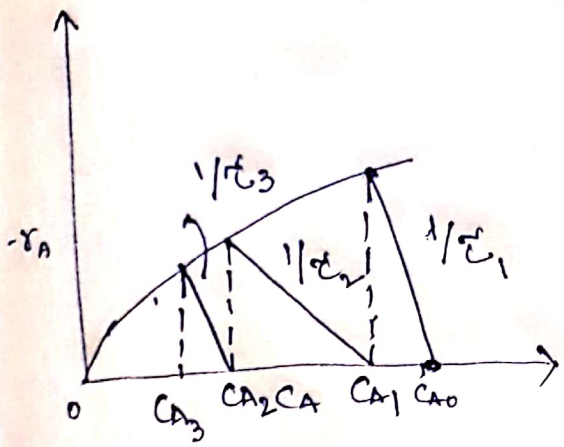
=> Assuming MFRs in series :—



We have $$\tau_1 = \frac{C_{A1} - C_{A0}}{-r_A}$$

or $$\frac{1}{\tau_1} = \frac{-r_A}{C_{A1} - C_{A0}} \quad \longrightarrow (6)$$

If we plot $-r_A$ v/s C_A



from (6)

$$\Rightarrow \frac{1}{\tau_1} = \frac{(-r_A)}{C_{A1} - C_{A0}} \quad \text{— for tank (1)}$$

$$\Rightarrow \frac{1}{\tau_2} = \frac{(-r_A)}{C_{A2} - C_{A1}} \quad \text{— for tank (2)}$$

$$\Rightarrow \frac{1}{\tau_3} = \frac{(-r_A)}{C_{A3} - C_{A2}} \quad \text{— for tank (3)}$$