

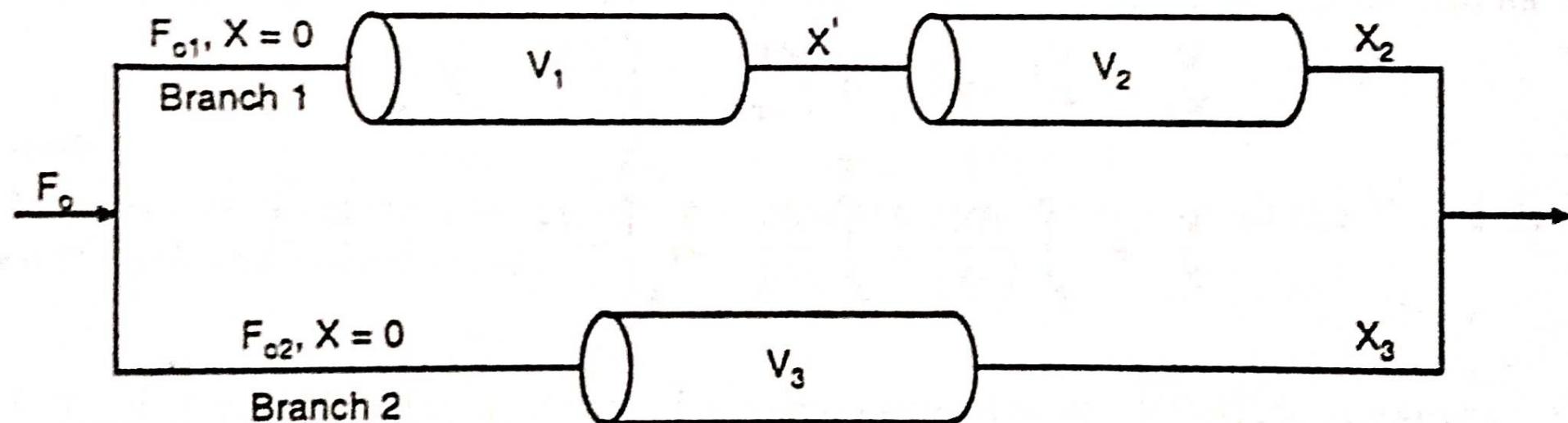
Multiple Reactors

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Plug Flow Reactors in Parallel

For plug flow reactors placed in parallel or any parallel-series combination V/F or τ must be same for each parallel line to have conversion to be the same in each branch. In case of parallel-series combination, the reactors in series are to be treated as a single reactor having a volume equal to the sum of volumes of reactors in series.

Consider a reactor set-up consisting of three PFRs in two branches as shown in Fig. 4.16. Branch-1 is having a reactor of volume V_1 followed by a reactor of volume V_2 . Branch-2 has a reactor of volume V_3 .



Branch-1 consists of two PFRs in series, hence the system of two PFRs in series may be considered as a single reactor of volume V.

$$V = V_1 + V_2$$

For branch-1 :

$$\frac{V}{F_{o1}} = \int_0^{X_2} \frac{dX}{(-r)}$$

For branch-2 :

$$\frac{V_3}{F_{o2}} = \int_0^{X_3} \frac{dX}{(-r)}$$

For PFRs in parallel, V/F must be identical (same) if the conversion is to be the same in each branch.

Therefore, for $X_2 = X_3 = X$

$$\frac{V}{F_{o1}} = \frac{V_3}{F_{o2}}$$

and

$$F_o = F_{o1} + F_{o2}$$

Assuming $V_1 = 40 \text{ l}$, $V_2 = 20 \text{ l}$ and $V_3 = 30 \text{ l}$ then what fraction of the feed should go to branch-1 for the conversion to be the same in each branch.

For branch-1,

$$\begin{aligned}V &= \text{total volume of two reactors} \\&= 40 + 20 = 60 \text{ l}\end{aligned}$$

$$F_{o1} = \text{Feed rate}$$

For reactors in parallel, V/F must be identical if the conversion is to be the same in each branch.

∴

$$\left(\frac{V}{F}\right)_1 = \left(\frac{V}{F}\right)_2$$

$$\frac{60}{F_{o1}} = \frac{30}{F_{o2}}$$

$$F_{o1} = 2 F_{o2}$$

We have

$$F_o = F_{o1} + F_{o2}$$

$$F_o = 2 F_{o2} + F_{o2}$$

$$F_{o2} = \frac{1}{3} F_o$$

and

$$F_{o1} = \left(1 - \frac{1}{3}\right) F_o$$

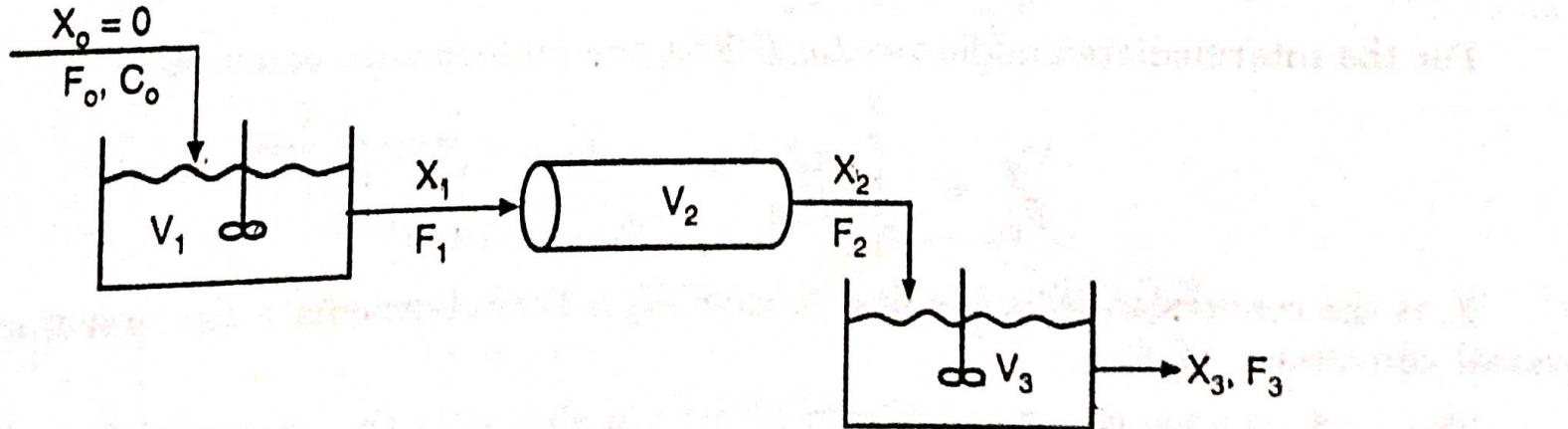
$$F_{o1} = \frac{2}{3} F_o$$

∴ Two-thirds of the feed must be fed to branch-1.

Case-1 CSTR followed by plug flow reactor followed by CSTR

Reactors of different types in series :

Consider a system of reactors in series as shown in the figure in which a mixed flow reactor/CSTR is followed by a PFR (plug flow reactor) which is followed by another CSTR.



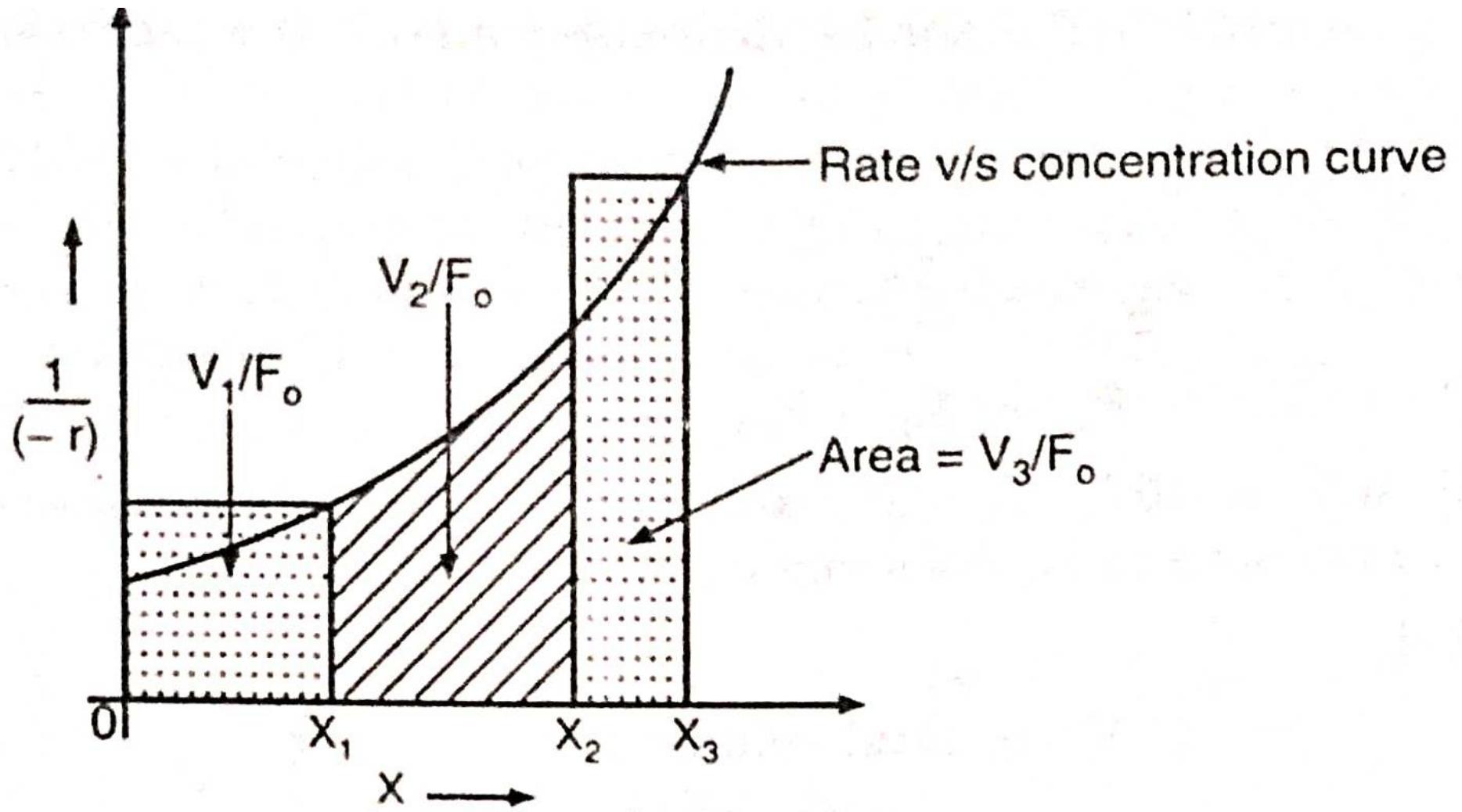
For the reactor sequences shown in the figure, the relationships between conversion and molar flow rates are shown below:

$$F_1 = F_0 - F_0 X_1 = F_0(1 - X_1)$$

$$F_2 = F_0(1 - X_2)$$

$$F_3 = F_0(1 - X_3)$$

$$X_2 = \frac{\text{total moles of A reacted upto point 2}}{\text{moles of A fed to first reactor}}$$



Graphical representation of series reactors

A material balance (on the mole basis) of species A for the CSTR at the end of our reactor system gives

$$\text{in} = \text{out} + \text{disappearance}$$

$$F_2 = F_3 + (-r)_3 V_3$$

Rearranging gives

$$V_3 = \frac{F_2 - F_3}{(-r)_3}$$

The corresponding rate of reaction $(-r)_3$ is evaluated at the conversion X_3 .

Similarly, for the first reactor (CSTR), the performance equation is

$$\frac{V_1}{F_0} = \frac{X_1 - X_0}{(-r)_1}$$

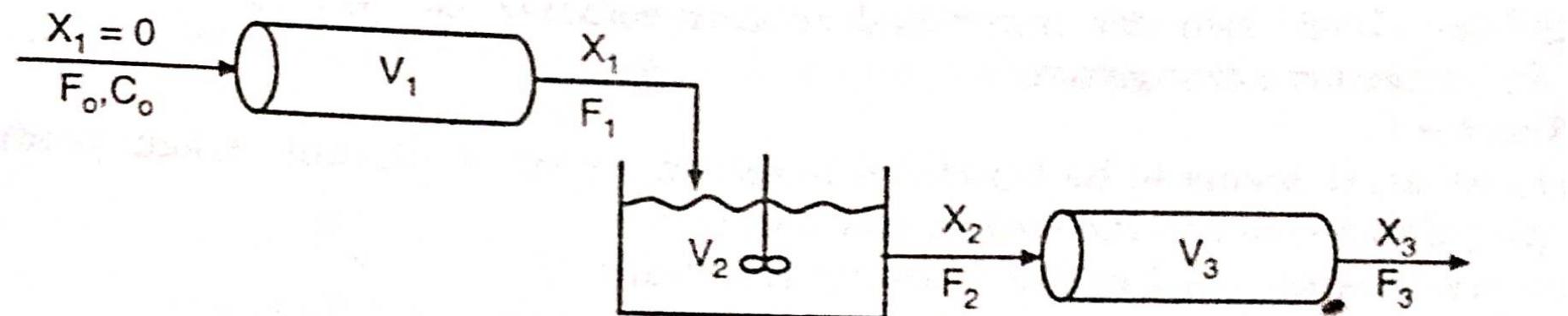
For the intermediate/middle reactor (PFR), the performance equation is

$$\frac{V_2}{F_0} = \int_{X_1}^{X_2} \frac{dX}{(-r)}$$

X_1 is the conversion from the first reactor, X_2 is the intermediate conversion and X_3 is the overall conversion of A.

The performance equations/relationships are shown in the graphical form in figure which will be helpful to us to predict the intermediate conversions as well as the overall conversion from the reactor system as a whole (i.e., all reactors in series).

Case-2 Plug Flow reactor followed by CSTR followed by plug flow reactor



Plug flow reactor followed by CSTR followed by plug flow reactor

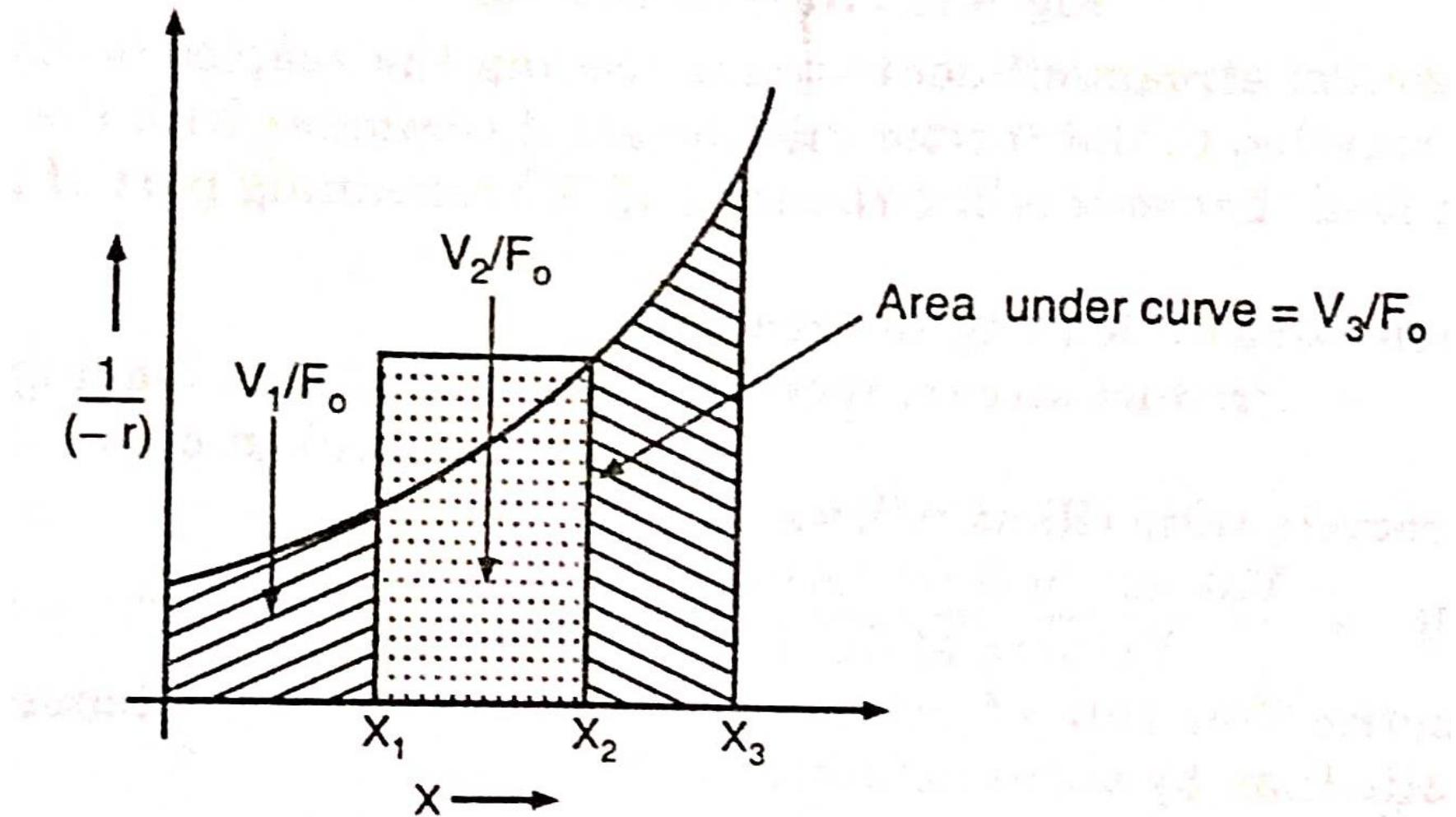
$$\frac{V_1}{F_0} = \int_{X_0}^{X_1} \frac{dX}{(-r)}$$

$$\frac{V_2}{F_0} = \frac{X_2 - X_1}{(-r)_2}$$

$$\frac{V_3}{F_0} = \int_{X_2}^{X_3} \frac{dX}{(-r)}$$

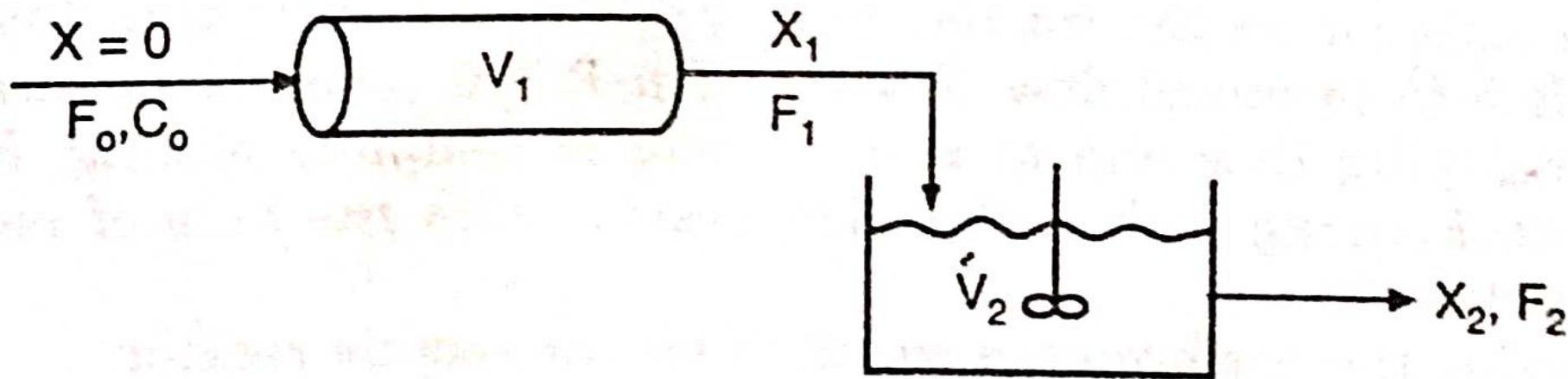
V_1 , V_2 , and V_3 are the volume of the reactors. F_0 is the flow rate which is same for both the reactors

Graphical Design Procedure

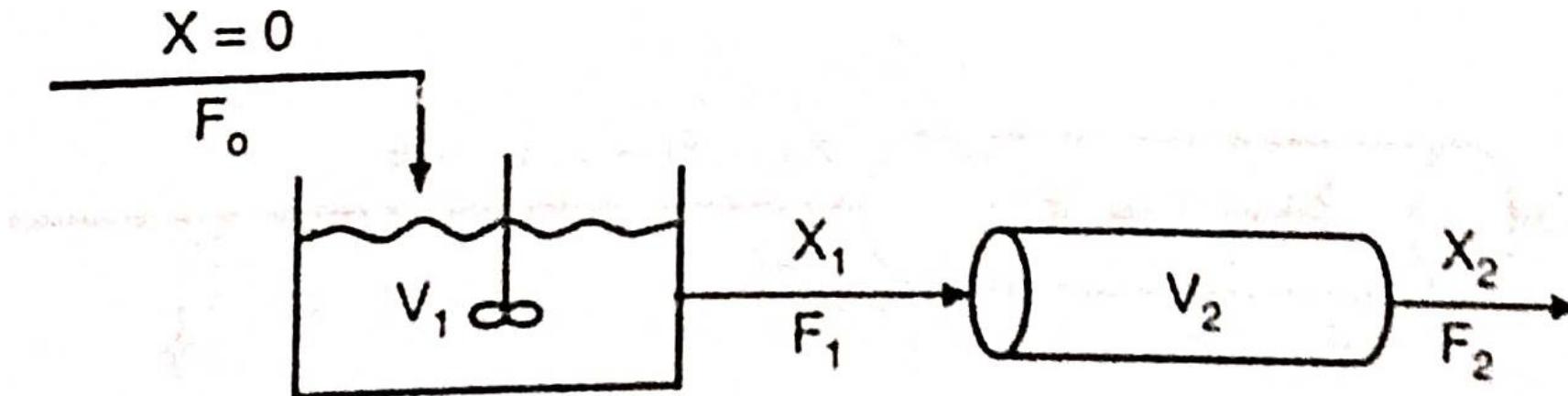


- Consider a CSTR is connected to a PFR. There are two ways in which they may be connected in series.

Scheme-1 PFR followed by CSTR



Scheme-2 CSTR followed by PFR

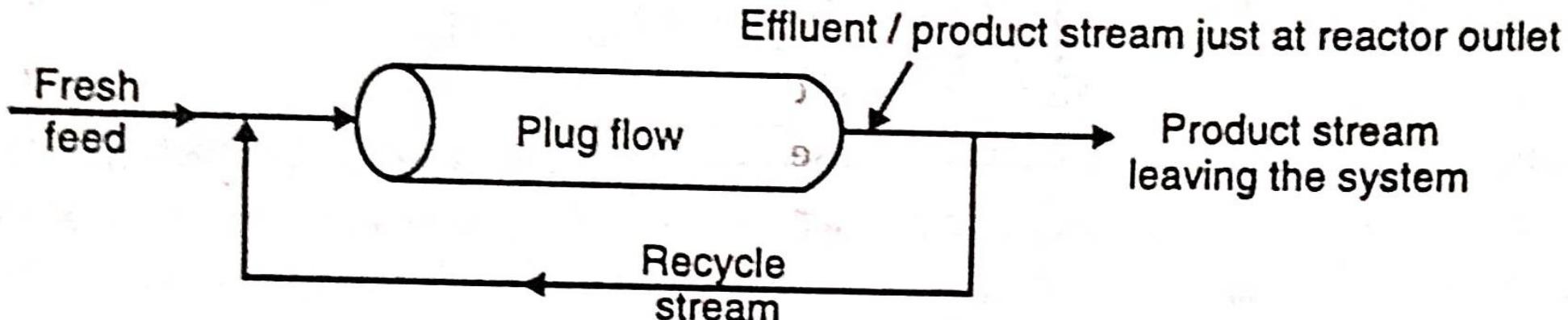


If the size of the reactors are fixed , then a different conversion will be obtained depending on which reactor is placed first.

- If the intermediate and overall conversion are fixed the individual reactor volumes as well as total reactor volume will be different depending on the arrangements

Recycle Reactor

- In some cases, it is beneficial to return a part of the effluent or product stream to the feed.
- Recycle reactors are used in the following situations:
 - (i). When the reaction is autocatalytic.
 - (ii). When it is required to maintained isothermal operation.
 - (iii). When it is necessary to promote a certain selectivity of a product.



Recycle Ratio

- Product/effluent stream leaving the reactor is divided into two streams
 - (i) One part is recycled to the reactor inlet and mixed with the fresh feed.
 - (ii) Second part is take out as product.

We define Recycle Ration (R) as

$$R = \frac{\text{Volume of fluid returned to the reactor inlet in feed}}{\text{Volume of fluid leaving the reactor as product}}$$

Recycle reactor different flows

If v_f = volumetric flow rate of product stream leaving the system

$$\text{Volumetric flow rate of recycle stream} = R \cdot v_f$$

Volumetric flow rate product stream exiting the reactor

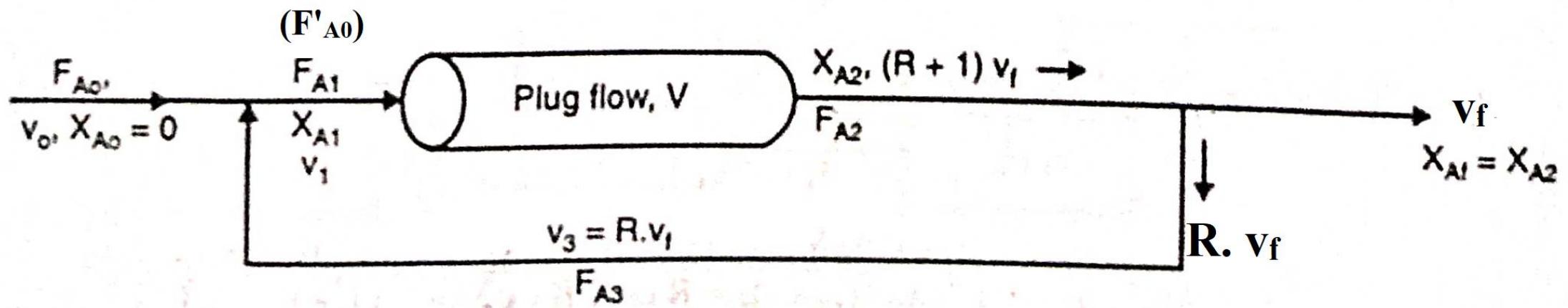
$$= R \cdot v_f + v_f = (R + 1)v_f$$

Recycle ration can vary from zero(PFR) to infinity, ∞ , (mixed reactor).

For $R=0$, there is no mixing.

For $R=\infty$, there is complete mixing.

Consider a recycle reactor with notations described in the following figure for developing performance of recycle reactor



For plug flow reactor, the performance equation for partially converted feed based upon the molar flow rate of A with no conversion(molar flow rate of unconverted A)

$$\frac{V}{F'_{A_0}} = \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{(-r_A)}$$

Where, F'_{A_0} = hypothetical feed of A in the mixed feed to the reactor with no conversion (fresh feed plus recycle feed without **conversion**) and

F'_{A_0} = hypothetical flow rate in converted stream in the mixed feed for a conversion of X_{A1} .

$$F'_{A_0} = \left(\text{A in fresh feed} \right) + \left(\begin{array}{l} \text{A in an} \\ \text{unconverted} \\ \text{recycle stream} \end{array} \right)$$

$$= F_{A_0} + R F_{A_0}$$

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

$$(A \text{ in an unconverted}) = v_3 C_{A0} = R v_f C_{A0} = R v_o C_{A0} = R F_{A0}$$

(recycle stream)

To get X_{A1} in terms of known quantities, we may write

$$X_{A1} = \frac{1 - C_{A1}/C_{A0}}{1 + e_A C_{A1}/C_{A0}}$$

For constant pressure throughout, we have

$$\begin{aligned} C_{A1} = \frac{F_{A1}}{v_1} &= \frac{F_{A0} + F_{A3}}{v_0 + R v_f} = \frac{F_{A0} + R F_{A0} (1 - X_{Af})}{v_0 + R v_o (1 + e_A X_{Af})} \\ &= C_{A0} \left[\frac{1 + R (1 - X_{Af})}{1 + R (1 + e_A X_{Af})} \right] = C_{A0} \left[\frac{1 + R - R X_{Af}}{1 + R + R e_A X_{Af}} \right] \end{aligned}$$

$$\therefore \frac{C_{A1}}{C_{A0}} = \left[\frac{1 + R - R X_{Af}}{1 + R + R e_A X_{Af}} \right]$$

Putting this value of C_{A1}/C_{A0} in equation (4.58) gives

Putting this value of $\frac{C_{A1}}{C_{A0}}$

$$X_{A1} = \frac{1 - \left[\frac{(1 + R - RX_{Af})}{1 + R + R\epsilon_A X_{Af}} \right]}{1 + \epsilon_A \left[\frac{1 + R - RX_{Af}}{1 + R + R\epsilon_A X_{Af}} \right]}$$

$$= \frac{1 + R + R\epsilon_A X_{Af} - 1 - R + RX_{Af}}{1 + R + R\epsilon_A X_{Af} + \epsilon_A + R\epsilon_A - R\epsilon_A X_{Af}} = \frac{R(1 + \epsilon_A) X_{Af}}{(1 + \epsilon_A) + R(1 + \epsilon_A)}$$

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

$$X_{A1} = \left(\frac{R}{R + 1} \right) X_{Af}$$

$$\frac{V}{F_{A_0}(R+1)} = \left(\frac{R}{R+1} \right) \int_{X_{A_0}}^{X_{A_f}} \frac{dX_A}{(-r_A)}$$

$$\frac{V}{F_{A_0}} = (R+1) \left(\frac{R}{R+1} \right) \int_{X_{A_0}}^{X_{A_f}} \frac{dX_A}{(-r_A)}, \text{ for any } \varepsilon_A$$

For constant density process above equation can be written in terms of concentration. The performance equation for PFR In terms of concentration.

$$\tau = \frac{C_{A_0} V}{F_{A_0}} = - \int_{C_{A_0}}^{C_{A_f}} \frac{dC_A}{(-r_A)}$$

Performance equation in terms of concentration for $\varepsilon_A = 0$

$$\tau = \frac{C_{A0} V}{F_{A0}} = - \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{(-r_A)} \quad \dots \text{for } \varepsilon_A = 0$$

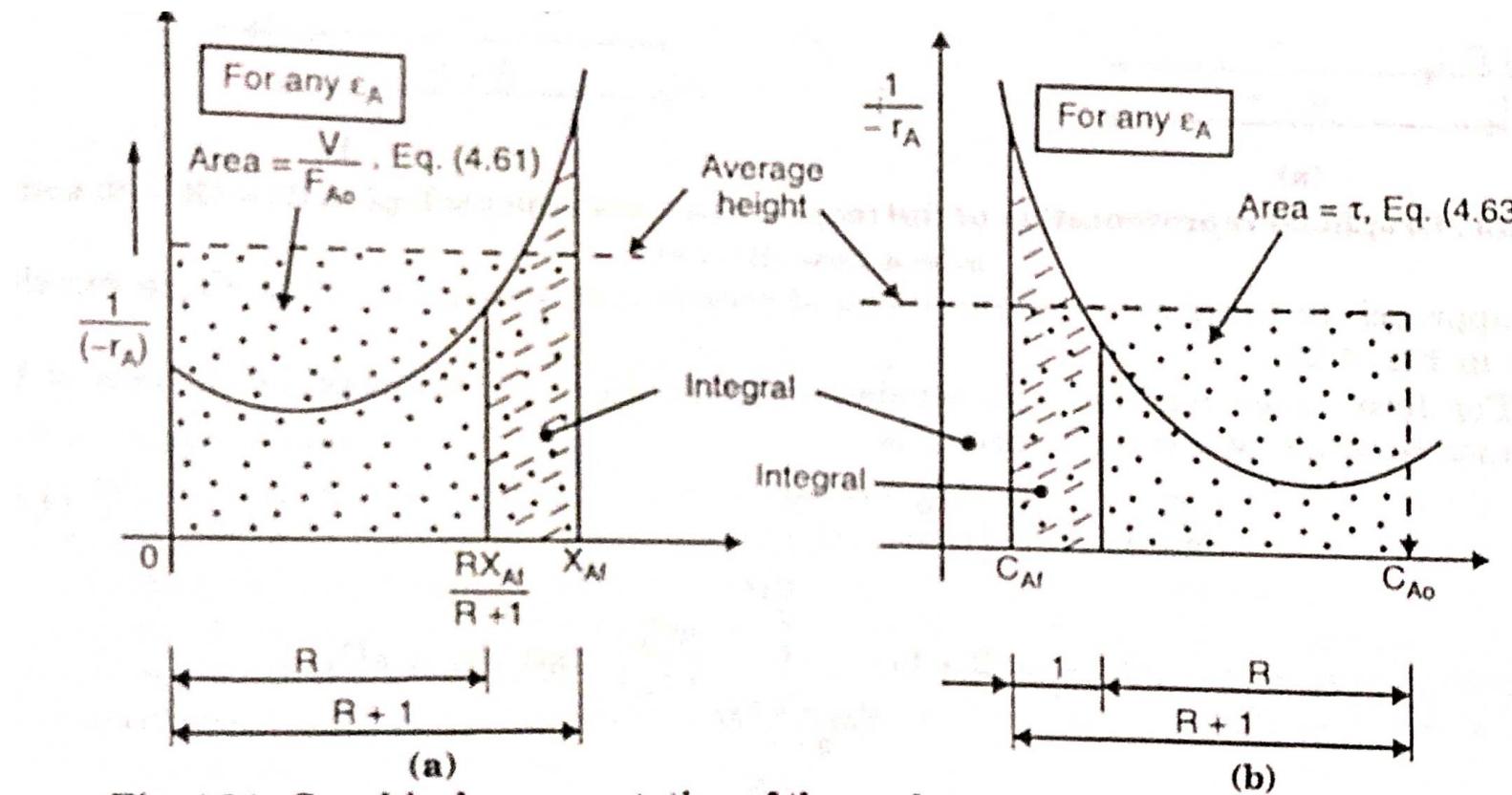
$$\begin{aligned} C_{A1} &= \frac{F_{A1}}{V_1} = \frac{F_{A0} + F_{A3}}{V_0 + V_S} = \frac{F_{A0} + R F_{A0} (1 - X_{Af})}{V_0 + R V_f} \\ &= \frac{F_{A0} + R F_{A0} (1 - X_{Af})}{V_0 + R V_0}, \quad V_0 = V_f \text{ for } \varepsilon_A = 0 \\ &= \frac{F_{A0}}{V_0} \left[\frac{1 + R (1 - X_{Af})}{R + 1} \right] \\ &= \frac{C_{A0} [1 + R (1 - X_{Af})]}{(R + 1)} = \frac{C_{A0} + R C_{A0} (1 - X_{Af})}{(R + 1)} \end{aligned}$$

but $C_{Af} = C_{A0} (1 - X_{Af})$

$$C_{A1} = \frac{C_{A0} + R C_{Af}}{R + 1}$$

$$\tau = \frac{C_{A_0} V}{F_{A_0} (R + 1)} = - \frac{\int_{C_{A_0}}^{C_{A_f}} \frac{dC_A}{(-r_A)}}{C_{A_0} + R C_{A_f}} \quad \dots \text{for } \varepsilon_A \neq 0$$

$$\tau = \frac{C_{A_0} V}{F_{A_0}} = -(R + 1) \frac{\int_{C_{A_0}}^{C_{A_f}} \frac{dC_A}{(-r_A)}}{C_{A_0} + R C_{A_f}} \quad \dots \text{for } \varepsilon_A = 0$$



For the extreme conditions of recycle, i.e R=0 to R= ∞ ,
the recycle system approaches plug flow and mixed flow respectively.

We have :

$$\frac{V}{F_{A0}} = (R + 1) \int_{\left(\frac{R}{R+1}\right) X_{Af}}^{X_{Af}} \frac{dX_A}{(-r_A)}$$

For R = 0, it becomes

$$\frac{V}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \dots \text{plug flow equation}$$

For R = ∞ , it becomes

$$\frac{V}{F_{A0}} = \frac{X_{Af}}{(-r_A)_f} \dots \text{mixed flow equation}$$

Two extreme conditions

We have :

$$\frac{V}{F_{Ao}} = (R + 1) \int_{\left(\frac{R}{R+1}\right) X_{Af}}^{X_{Af}} \frac{dX_A}{(-r_A)}$$

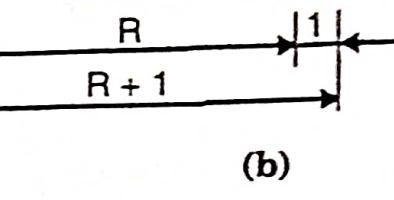
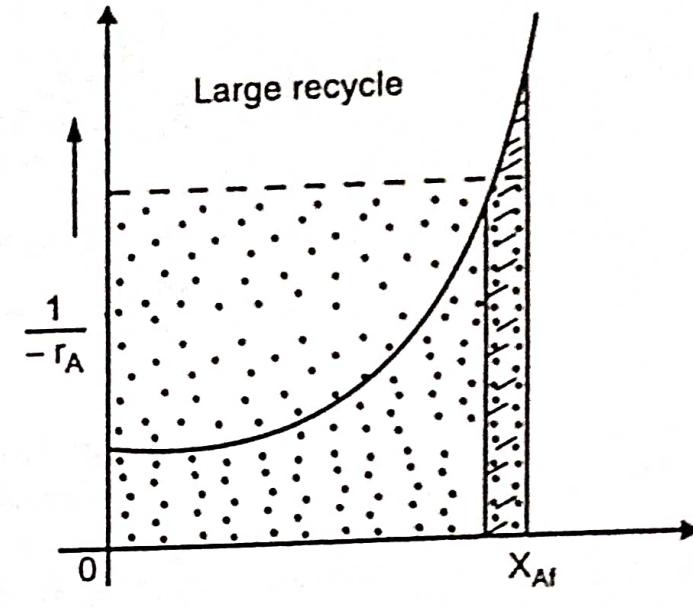
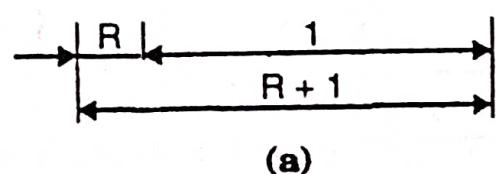
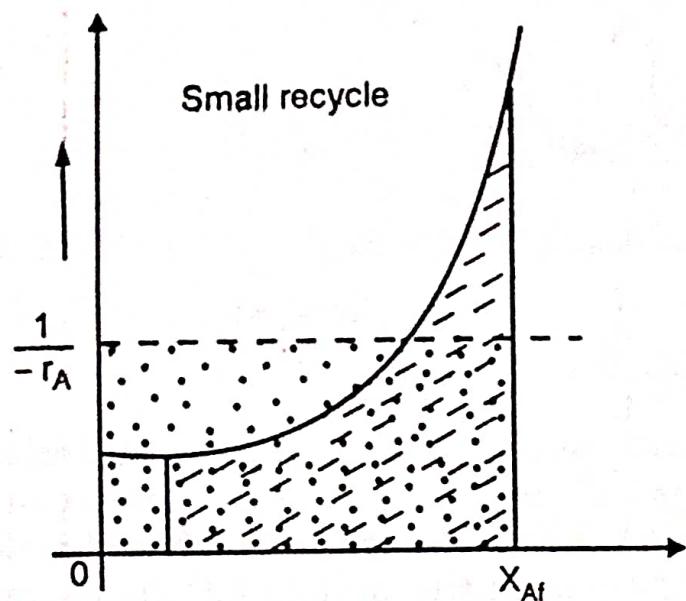
For $R = 0$, it becomes

$$\frac{V}{F_{Ao}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \dots \text{plug flow equation}$$

For $R = \infty$, it becomes

$$\frac{V}{F_{Ao}} = \frac{X_{Af}}{(-r_A)_f} \dots \text{mixed flow equation}$$

Graphical presentation for $R=0$ to $R=\infty$,



For first order reaction and constant density, $\varepsilon_A = 0$

$$\frac{k\tau}{R+1} = \ln \left[\frac{C_{A_0} + R C_{Af}}{(R+1) C_{Af}} \right]$$

$$\tau = -(R+1) \int_{\frac{C_{A_0} + R C_{Af}}{(R+1)}}^{C_{Af}} \frac{dC_A}{(-r_A)} \quad \text{and} \quad -r_A = kC_A$$

$$\tau = -(R+1) \int_{\frac{C_{A_0} + R C_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{kC_A}$$

$$= \frac{-(R+1)}{k} [\ln C_A]_{\frac{C_{A_0} + R C_{Af}}{R+1}}^{C_{Af}} = \frac{(R+1)}{k} \ln \left[\frac{C_{A_0} + R C_{Af}}{(R+1) C_{Af}} \right]$$

$$\frac{k\tau}{R+1} = \ln \left[\frac{C_{A_0} + R C_{Af}}{(R+1) C_{Af}} \right]$$

For second order reaction and constant density, $\varepsilon_A = 0$

$$-r_A = k C_A^2$$

$$\tau = -(R + 1) \int_{\frac{C_{A0} + R C_{Af}}{R + 1}}^{C_{Af}} \frac{dC_A}{k C_A^2}$$

$$= \frac{-(R + 1)}{k} \left[-\frac{1}{C_A} \right]_{\frac{C_{A0} + R C_{Af}}{R + 1}}^{C_{Af}}$$

$$= \frac{(R + 1)}{k} \left[\frac{1}{C_{Af}} - \frac{R + 1}{C_{A0} + R C_{Af}} \right]$$

$$= \frac{(R + 1)}{k} \left[\frac{C_{A0} + R C_{Af} - R C_{Af} - C_{Af}}{(C_{A0} + R C_{Af}) C_{Af}} \right]$$

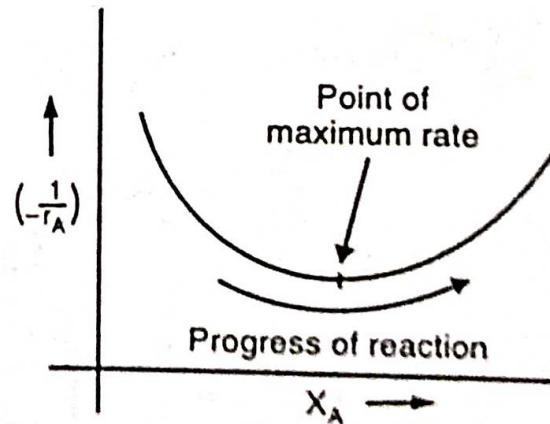
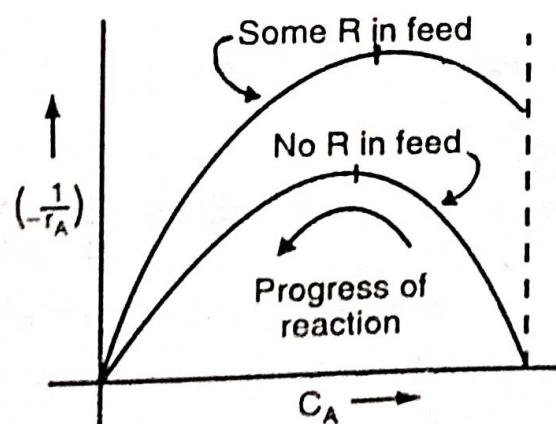
$$= \left(\frac{R + 1}{k} \right) \left[\frac{C_{A0} - C_{Af}}{C_{Af} (C_{A0} + R C_{Af})} \right]$$

$$\frac{\tau k}{R + 1} = \frac{(C_{A0} - C_{Af})}{C_{Af} (C_{A0} + R C_{Af})}$$

$$\frac{\tau k C_{A0}}{R + 1} = \frac{C_{A0} (C_{A0} - C_{Af})}{C_{Af} (C_{A0} + R C_{Af})}$$

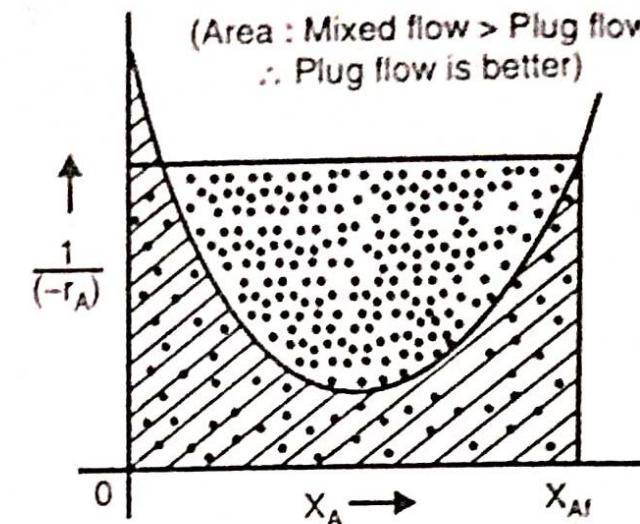
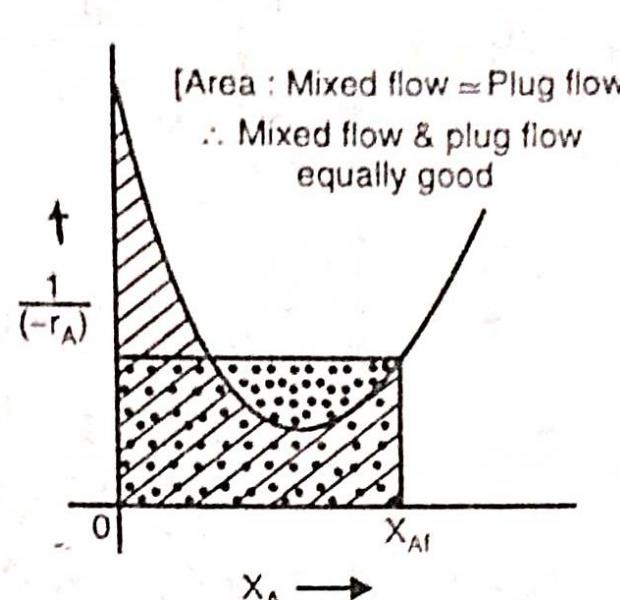
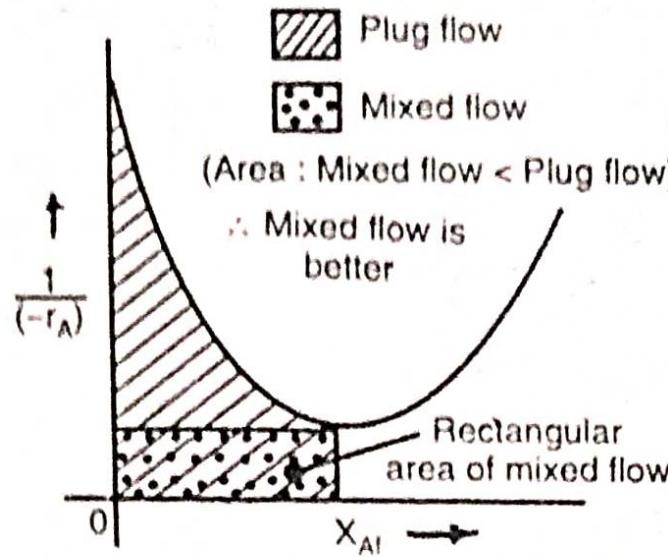
Autocatalytic Reactions :

When reactant A reacts by any n^{th} order rate ($n > 0$) in a batch reactor, its rate of disappearance is fast at the start due to its higher initial concentration. As the reactant get consumed, this rate decreases progressively. In autocatalytic reactions, however, the rate of reaction at the start is low for the reason that little product is present initially. This rate increases to the maximum as product is formed and then decreases progressively to a low value as the reactant is consumed by the reaction. The rate-concentration curve for ordinary n^{th} order autocatalytic reactions



Plug flow versus mixed flow reactor with no recycle for autocatalytic reaction

- For this reaction, we should have $(1/-r_A)$ vs. concentration plot or $(1/-r_A)$ vs. conversion plot .
- Then comparing the area we can choose the best type of reactor.



Comparison of area.

- At low conversion mixed flow reactor is superior to the plug flow reactor.
- At higher conversion, plug flow reactor is superior to the mixed flow reactor.
- For ordinary nth order reaction, $n > 0$, plug flow reactor is more efficient than that of mixed flow reactor.

Optimum recycle ratio.

When we process materials in a recycle reactor to achieve some fixed conversion there is a certain recycle ratio which is optimum. By the optimum recycle ratio we mean the recycle ratio with which we need a minimum reactor volume.

The optimum recycle ratio is obtained by differentiating equation (4.61) with respect to R and setting $\frac{d(V/F_{A_0})}{dR}$ to zero.

We have :

$$\frac{V}{F_{A_0}} = (R + 1) \int_{\left(\frac{R}{R+1}\right) X_{A_i}}^{X_{A_f}} \frac{dX_A}{(-r_A)}$$

$$\therefore \frac{V}{F_{A_0}} = \frac{\tau}{C_{A_0}} = \int_{X_{A_i} = \frac{R X_{A_f}}{R+1}}^{X_{A_f}} \frac{(R+1)}{(-r_A)} dX_A$$

Differentiate τ/C_{A_0} w.r.t, R and set $\frac{d(\tau/C_{A_0})}{dR} = 0$

This operation requires differentiating under an integral sign.

If

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

By applying calculus

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

$$\frac{d(\tau/C_{A_0})}{dR} = 0 = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)} + 0 - \left. \frac{R+1}{(-r_A)} \right|_{X_{Ai}} \frac{dX_i}{dR}$$

$$\int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)} = \left. \frac{(R+1)}{(-r_A)} \right|_{X_{Ai}} \cdot \frac{dX_{Ai}}{dR}$$

We have,

$$X_{Ai} = \left(\frac{R}{R+1} \right) X_{Af}$$

$$\frac{dX_{Ai}}{dR} = X_{Af} \left[\frac{(R+1) \times 1 - R \times 1}{(R+1)^2} \right]$$

$$\frac{dX_{Ai}}{dR} = \frac{X_{Af}}{(R+1)^2}$$

$$X_{Af} - X_{Ai} = X_{Af} - \left(\frac{R}{R+1} \right) X_{Af}$$

$$(X_{Af} - X_{Ai}) = X_{Af} \left[1 - \frac{R}{R+1} \right] = \frac{X_{Af}}{(R+1)}$$

$$\therefore \left. \frac{1}{(-r_A)} \right|_{X_{Ai}} \times (X_{Af} - X_{Ai}) = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)}$$

\therefore For the optimum, we have

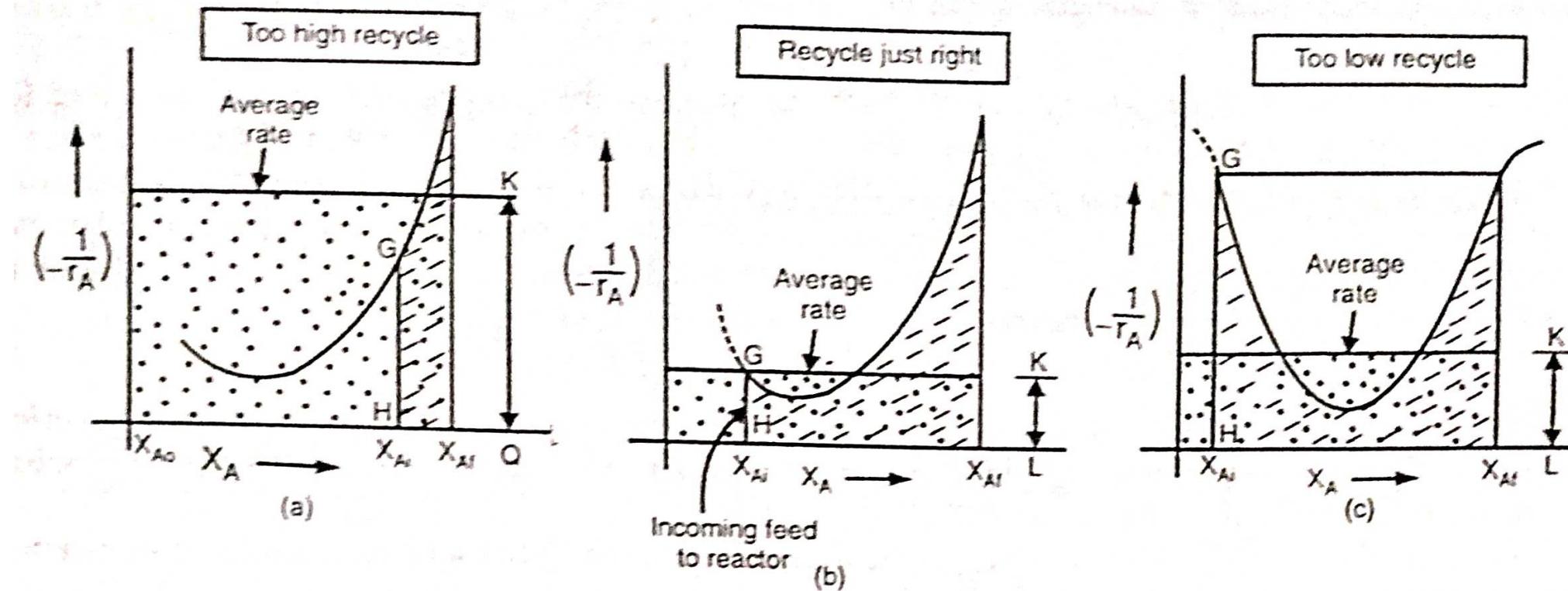
$$\left. \frac{1}{(-r_A)} \right|_{X_{Ai}} = \frac{\int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)}}{(X_{Af} - X_{Ai})}$$

Where, X_{Ai} is calculated from $X_{Ai} = \frac{R}{R+1} X_{Af}$

If at the feed condition, $1/-r_{Ai}$ is equal to the average value of $1/-r_A$ in the whole reactor

Then the corresponding recycle ratio will be the optimum.

Comparison of recycle ratios in autocatalytic reaction

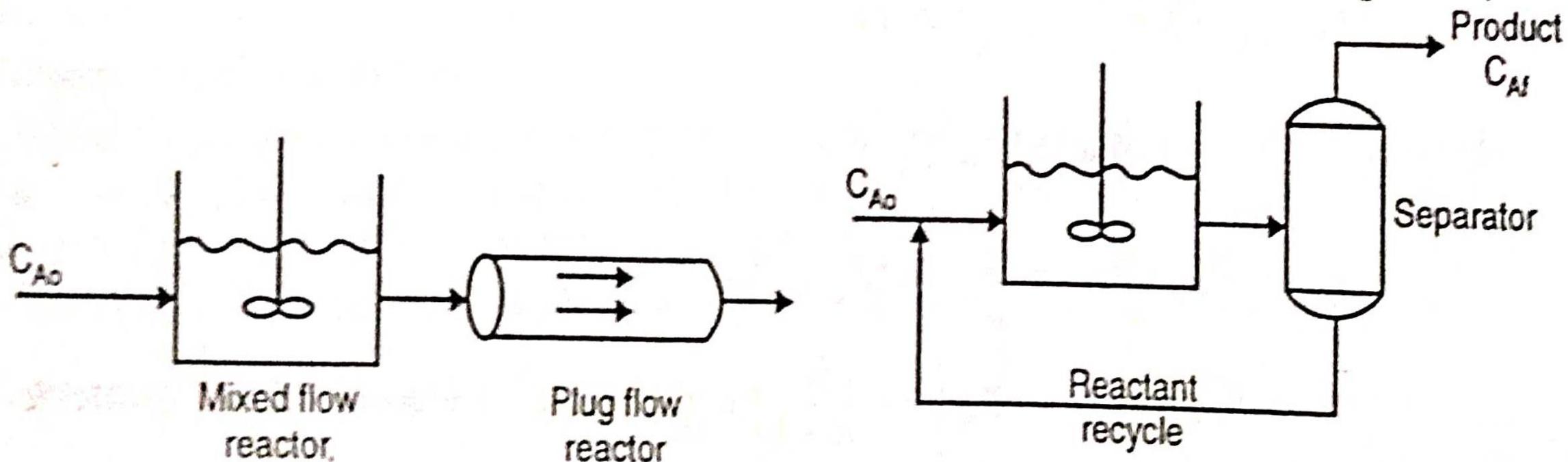


Examples of Autocatalytic Reactions:

(i) Fermentation reactions which involve the action of microorganism on an organic feed, (ii) Combustion of fuel gas occurring in an adiabatic manner with a feed consisting of cool reactants to the system. Such combustion reactions are referred as autothermal because here heat is considered as the product which sustains the reaction and will die with plug flow and will be self-sustaining with backmix/mixed flow as the heat generated by the reaction can heat the fresh reactants to a temperature at which they will react.

Reactor Combinations for Autocatalytic reactions:

For carrying out autocatalytic reactions where product recycle or product separation with recycle is permissible, we have to consider all sorts of reactor arrangements. In general, when



By graphical analysis, the best arrangement of the reactors can be determined.

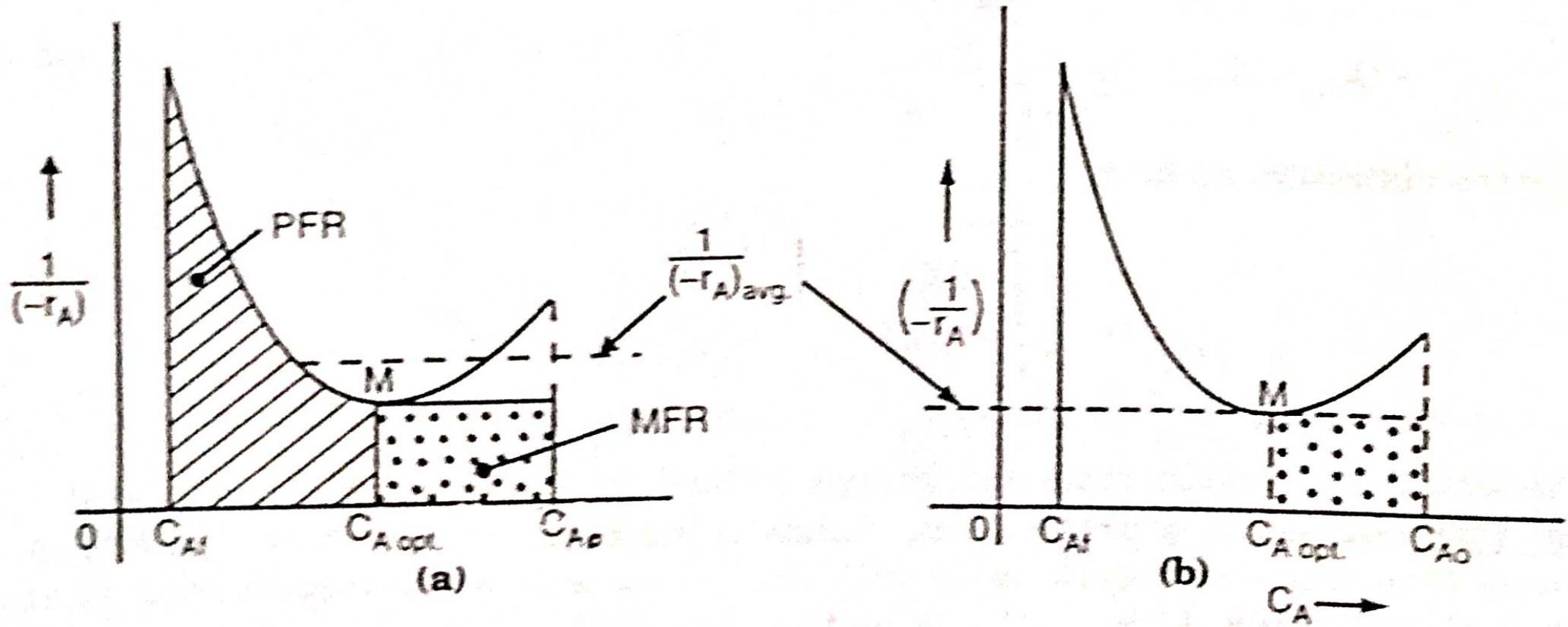


Fig. 4.29 : (a) The best multiple reactor scheme
 (b) The best scheme for separation and reuse (by recycle) of unconverted reactant