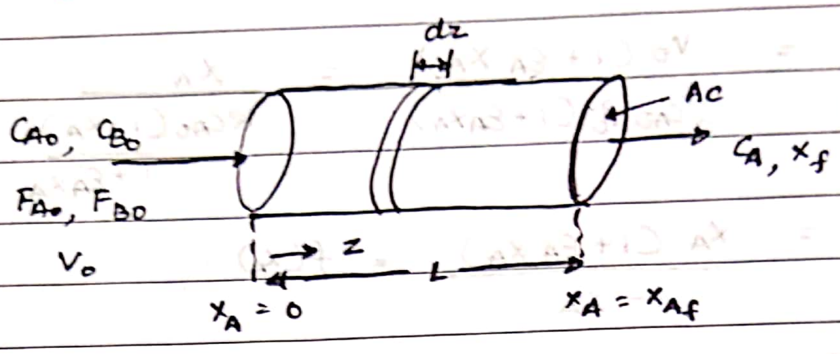
Plug Flow reactors



Mole Balance : $F_A = (F_A + dF_A) + (-r_A)\,dV$

$$-dF_A = -r_A\,dV \Rightarrow -\frac{dF_A}{dV} = -r_A$$

$$-r_A = \frac{k\,(P_A - P_R P_S)}{1 + K_A P_A + K_R P_R} \quad (A \rightarrow R + S)$$

Design of PFR

Volume Basis :

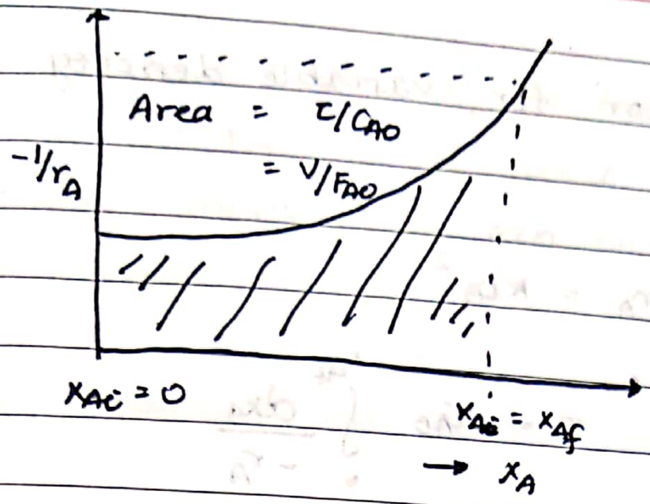
As, $F_A = F_{A0}(1 - X_A)$, $F_{A0}\dfrac{dX_A}{dV} = -r_A$

$$\frac{V}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \qquad \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

Catalyst weight basis

$$-\frac{dF_A}{dW} = -r_A'$$

$$\frac{W}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A'}$$



Plug Flow Reactor for variable Density with first order kinetics

Rate eqn : $-r_A = k C_A$

$$\tau = C_{A0} \int_{x_{Ai}}^{x_{Af}} \frac{(1+\varepsilon_A x_A)\, dx_A}{k C_{A0} (1-x_A)}$$

$$k\tau = \int_0^{x_A} \frac{dx_A}{1-x_A} + \varepsilon_A \int_0^{x_A} \frac{x_A\, dx_A}{1-x_A}$$

$$k\tau = -(1+\varepsilon_A) \ln(1-x_A) - \varepsilon_A x_A = (x_A)$$

For const. vol,

$\varepsilon_A = 0 \Rightarrow k\tau = -\ln(1-x_A) = (x_A)$

Plug flow reactor for variable density with 2nd order kinetics

Rate eqn : $-r_A = k C_A^2$

Mole Balance : $\tau = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A}$

$$\tau = C_{A0} \int_0^{X_{Af}} \frac{X_A (1+\varepsilon_A X_A)^2 \, dX_A}{k C_{A0}^2 (1-X_A)^2}$$

$$C_{A0} k \tau = 2\varepsilon_A (1+\varepsilon_A) \ln(1-X_A) \, \varepsilon_A^2 X_A + (1+\varepsilon_A)^2 \frac{X_A}{1-X_A}$$

$\tau = \frac{A_c L}{v_0}$, A_c is cross-section area.

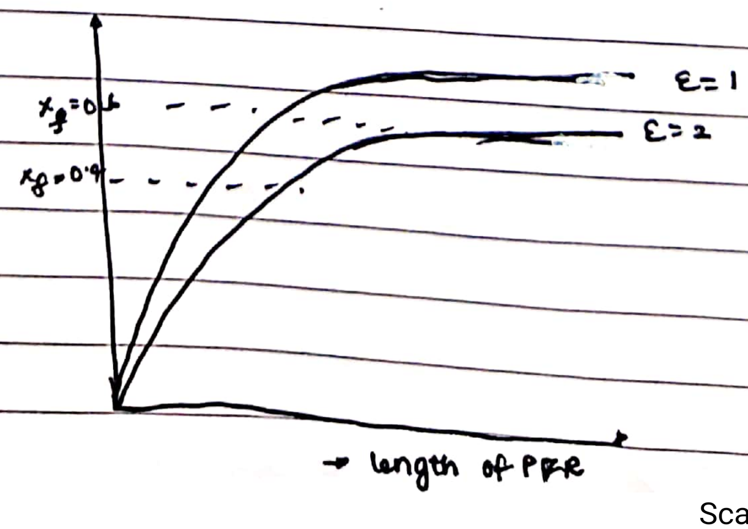
Conversion at diff. length

$$L = \frac{v_0}{C_{A0} k A_c} \left[2\varepsilon_A (1+\varepsilon_A) \ln(1-X_A) \, \varepsilon_A^2 X_A + (1+\varepsilon_A) \frac{X_A}{1-X_A} \right]$$

With increase of ε_A for same conversion, reactor length increases.

For const. reactor length, with increase of ε_A, conversion decreases.

Consider gas-phase rxn , $A \rightarrow 2B + C$, $\varepsilon_A = 2$



If we add 50% A, 50% N_2 as inert, $y_{A0} = 0.5$, then $\varepsilon_A = 2 \times 0.5 = 1$, this point will reside b/w $\varepsilon_A = 0$, $\varepsilon_A = 2$
so on adding inert, ε_A can be decreased, increasing conversion level.

Damköhler number for batch reactor

→ For batch reactor 'τ' will be replaced by t
For first order rxn, $k\tau = kt$
→ For batch reactor n-th order rxn, $C_{A0}^{n-1} kt$

Different Types of reactors

→ Batch Reactor
→ Flow Reactor
→ Multiple Reactors connected in series or parallel
→ Reactors with inter-stage feed injection
→ Recycling of Products to the Reactor.

Parameters for Reactor Selection

→ Cost of Reactor – (Most imp factor)
→ Capacity of Reactor
→ Time of Production
→ Safety consumption
→ Equipment life

Batch Reactor :

- → Small Instrument cost.
- → Flexibility of Operation
- → High labor and handling cost
- → Poorer quality of pdts.

These are suitable for small scale production
Time of batch op. is same as PFR for $\varepsilon_A = 0$, as

$$t = C_{A0} \int_0^{x_A} \frac{dx_A}{-r_A} = N_{A0} \int_0^{x_A} \frac{dx_A}{-r_A V}$$

$$\frac{V}{v_0} = \tau_p = C_{A0} \int_0^{x_A} \frac{dx_A}{-r_A}$$

Thus, for high flow reactors we prefer PFRs

Two flow reactors : Mixed and PFR should be compared.

Comparision between PFR and Mixed Reactor

let us consider the rate eqn:,

$$-r_A = \frac{1}{V}\frac{dN_A}{dt} = k C_A^n \quad (n \in [0, 3])$$

For mixed flow reactor,

$$\tau_m = \left(\frac{C_{A0} V}{F_{A0}}\right)_m = \frac{C_{A0} V}{-r_A} = \frac{1}{k C_{A0}^{n-1}} \frac{x_A (1+\varepsilon_A x_A)^n}{(1-x_A)^n}$$

Plug flow reactor,

$$\tau_p = \left(\frac{C_{A0} V}{F_{A0}}\right)_p = C_{A0} \int_0^{x_A} \frac{dx_A}{-r_A} = \frac{1}{k C_{A0}^{n-1}} \int_0^{x_A} \frac{x_A (1+\varepsilon_A x_A)^n}{(1-x_A)^n}$$

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$$\frac{\tau_m}{\tau_p} = \frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{(n-1)})_p} = \frac{\dfrac{x_A(1+\varepsilon_A x_A)^n}{(1-x_A)^n}}{\displaystyle\int_0^{x_A} \frac{x_A(1+\varepsilon_A x_A)^n}{(1-x_A)^n}\,dx_A}$$

For const. density system, $\varepsilon_A = 0$

$$\frac{\tau_m}{\tau_p} = \frac{V_M}{V_p} = \frac{\left(\dfrac{x_A}{(1-x_A)^n}\right)}{(-\ln(1-x_A))_p}$$

$\therefore$ Always $V_m > V_p$

→ $\frac{V_m}{V_p}$ increases with order

→ $\frac{V_m}{V_p}$ depends on ε_A

→ For zero order rxn., independent of type of reactors

Multiple Reactors

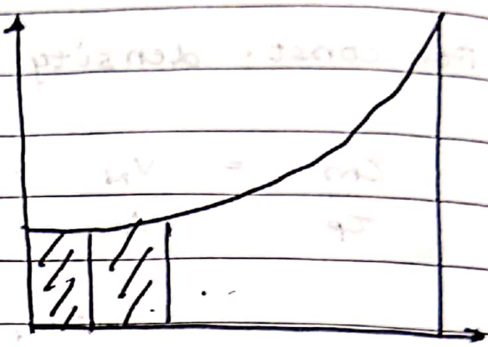
Plug flow reactors in series or parallel

Series Reactors

$$\frac{V}{F_0} = \sum_{i=1}^{N} \frac{V_i}{F_0} = \frac{V_1 + V_2 \cdots + V_N}{F_0}$$

$$\frac{V}{F_0} = \int_0^{X_{A1}} \frac{dX_A}{-r_A} + \cdots \int_{X_{N-1}}^{X_N} \frac{dX_A}{-r_A}$$

$$= \int_0^{X_N} \frac{dX_A}{-r_A}$$



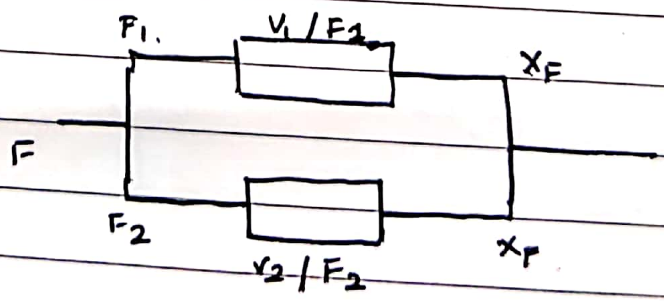
In a single sized reactor, $V = V_1 + V_2 + \cdots V_N$

Parallel reactors

Two mixed reactors are connected in parallel for $V_1 \neq V_2$,

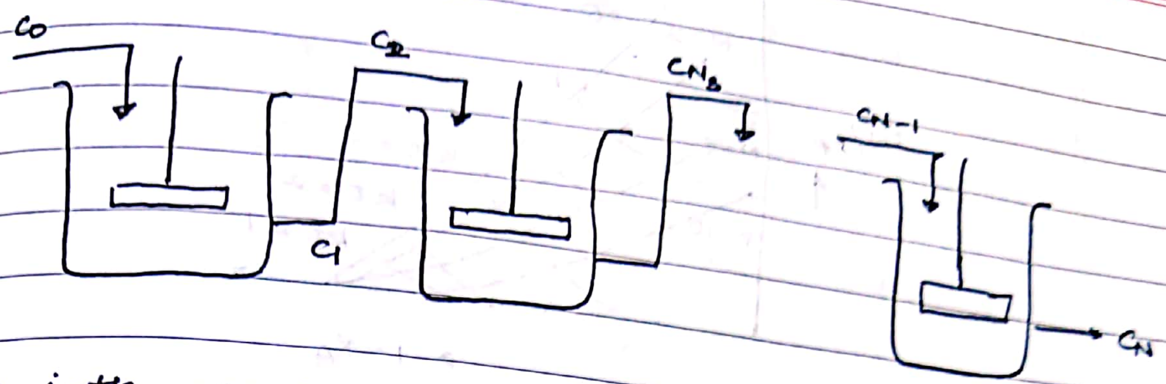
$$\frac{V_1}{F_1} = \frac{V_2}{F_2}$$

If $V_1/V_2 = 2 \Rightarrow F_1/F_2 = 2$



$\tau = \frac{V}{F}$ should be const. So final conversion at reactor outlet remain same.

CSTR in series



For i-th reactor,

$$\tau_i = \frac{C_0 V_i}{F_0} = \frac{V_i}{v} = \frac{C_0 (X_i - X_{i-1})}{-r_A}$$

$$\tau_i = \frac{C_0\left(\left[1 - \frac{C_i}{C_0}\right] - \left[1 - \frac{C_{i-1}}{C_0}\right]\right)}{-r_A} = \frac{C_{i-1} - C_i}{k C_i}$$

$$\frac{C_{i-1}}{C_i} = 1 + k\tau_i$$

$$\frac{C_0}{C_N} = \frac{C_0}{C_1} \cdot \frac{C_1}{C_2} \cdot \frac{C_2}{C_3} \cdots \frac{C_{N-1}}{C_N} = (1 + k\tau_i)^N$$

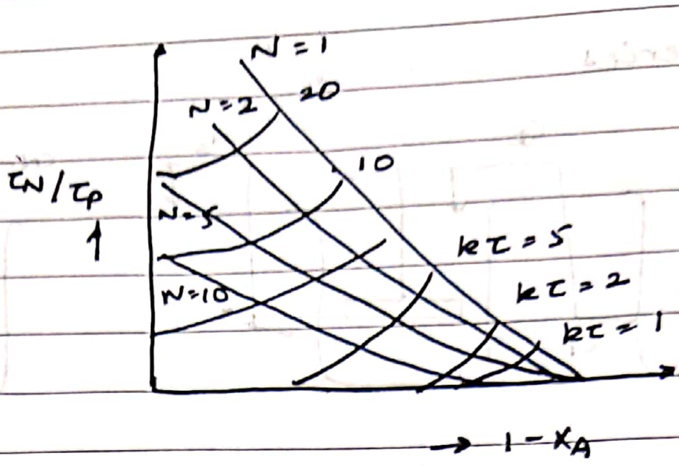
If $\tau_1 = \tau_2 = \tau_3 \cdots = \tau_i$

$$1 + k\tau_i = \left(\frac{C_0}{C_N}\right)^{1/N} \Rightarrow \tau_i = \frac{1}{k}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right]$$

$$\tau_m = \frac{N V_i}{v} = N\tau_i = \frac{N}{k}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right]$$

As $N \to \infty$, $\tau_p = \frac{1}{k} \ln \frac{C_0}{C}$, $\tau_m = \frac{1}{k} \ln \frac{C_0}{C_N}$

N-CSTR in series connection is converted to a plug flow reactor for $N \to \infty$



For first order rn., $\varepsilon = 0$ (N - CSTR)

When three reactors in series, (CSTR)

$$\tau_i = \frac{C_{i-1} - C_i}{-r_i}$$

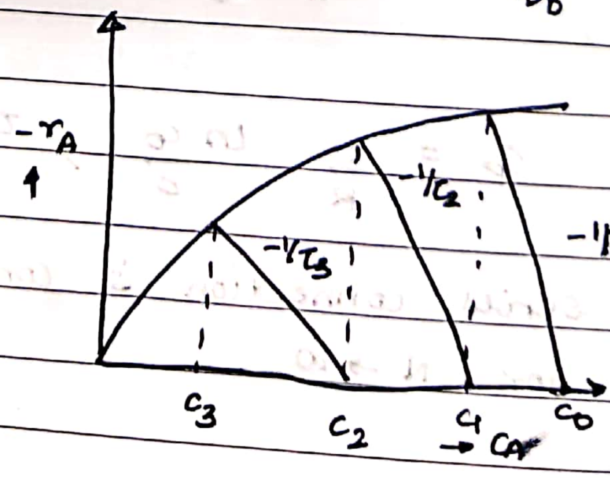
$i = 1, 2$ and 3

For R - 1, $-r_1 = \frac{-1}{\tau_1}(C_1 - C_0)$

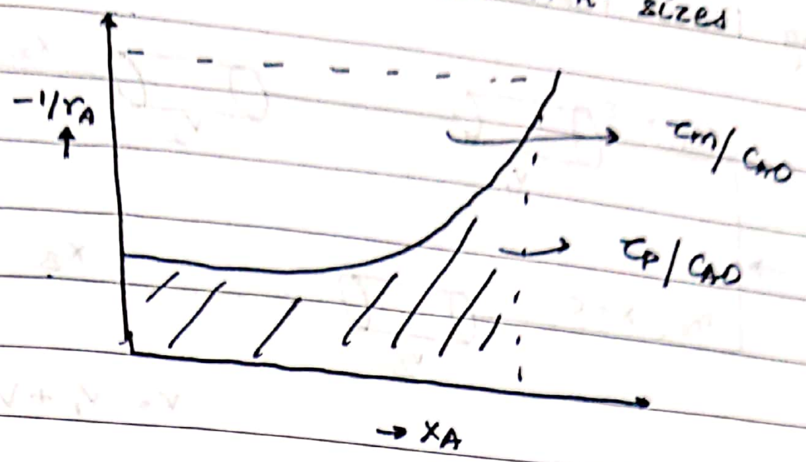
R - 2, $-r_2 = \frac{-1}{\tau_2}(C_2 - C_1)$

R - 3, $-r_3 = \frac{-1}{\tau_3}(C_3 - C_1)$

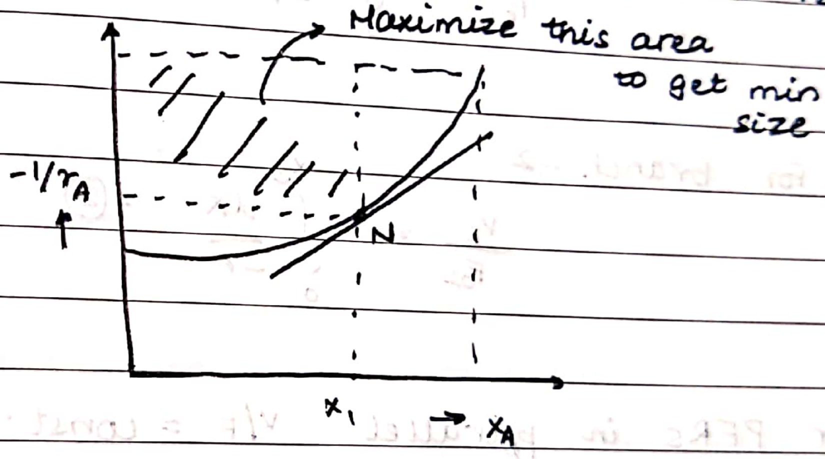
$\tau_1 = \frac{V_1}{v_0}$, $\tau_2 = \frac{V_2}{v_0}$, $\tau_3 = \frac{V_3}{v_0}$ → unequal sizes



Comparison between CSTR and PFR sizes



Finding Two minimum size of mixed flow reactors.



For first order rn:, $-r_A = kC_{A0}(1-X_A)$

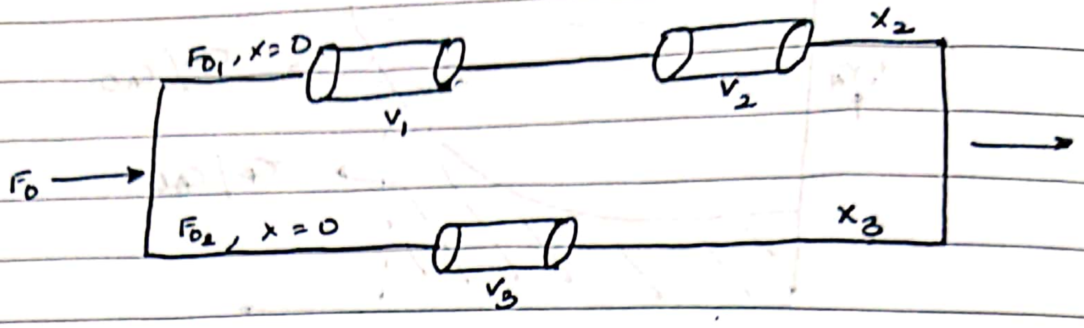
$A = xy \Rightarrow dA = y\,dx + x\,dy$

In this case, $y = -\frac{1}{r_A} = \frac{1}{kC_{A0}(1-X_A)}$

$\frac{y}{x} = \frac{1}{kC_{A0}(1-x_1)x_1} \Rightarrow \frac{dy}{dx} = \left.\frac{1}{kC_{A0}(1-X_A)^2}\right|_{X_A = X_1}$

$-\frac{dy}{dx} = \frac{y}{x}, \quad \frac{1}{kC_{A0}(1-X_1)^2} = \frac{1}{kC_{A0}(1-X_1)X_1} \Rightarrow X_1 = 0.5$

Plug Flow reactors in Parallel



$V = V_1 + V_2$

For branch - 1

$$\frac{V}{F_{01}} = \int_0^{x_2} \frac{dx}{-r} \quad - ①$$

For branch - 2

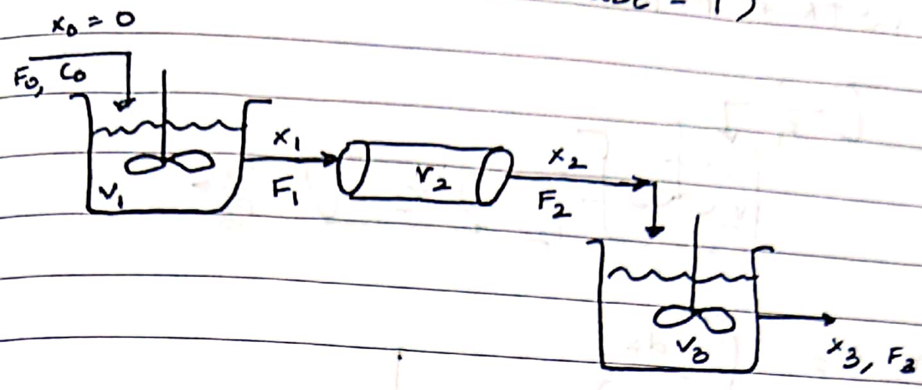
$$\frac{V_3}{F_{02}} = \int_0^{x_3} \frac{dx}{-r} \quad - ②$$

For PFRs in parallel V/F = const.

$\therefore \; x_2 = x_3 = x$

$$\frac{V}{F_{01}} = \frac{V}{F_{02}} \; ③ , \qquad F_0 = F_{01} + F_{02} \; ④$$

CSTR + PFR + CSTR (case - 1)

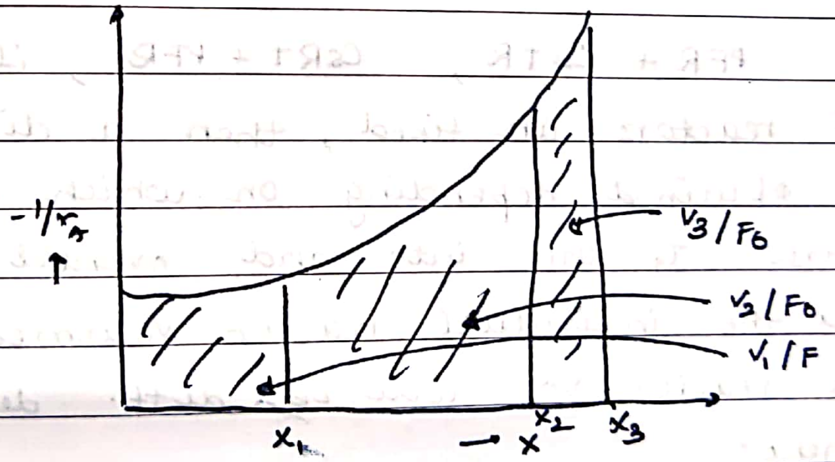


$F_1 = F_0 - F_0 x_1 = F_0 (1 - x_1)$

$F_2 = F_0 (1 - x_2)$

$F_3 = F_0 (1 - x_3)$

$x_2 = \dfrac{\text{Total moles of reacted till 2}}{\text{Moles of A fed to first reactor}}$



Material balance, $F_2 = F_3 + (-r_3) V_3$ (3rd reactor)

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

For 1st CSTR, $\dfrac{V_1}{F_0} = \dfrac{X_1 - x_0}{(-r)_1}$

For PFR, $\dfrac{V_2}{F_0} = \displaystyle\int_{x_1}^{x_2} \dfrac{dx}{-r}$

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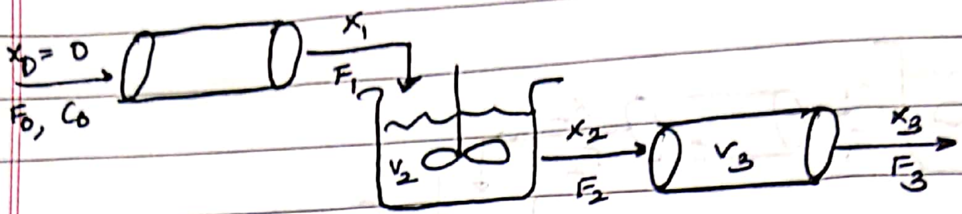
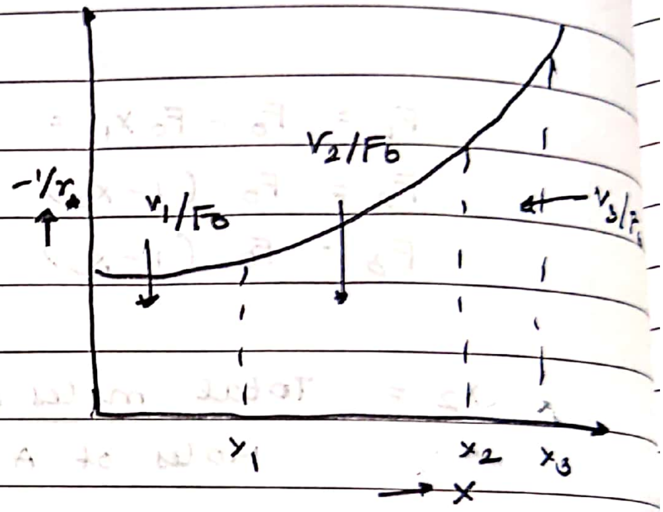
PFR + CSTR + PFR (Case - 2)



$$\frac{V_1}{F_0} = \int_{x_0}^{x_1} \frac{dx}{(-r)}$$

$$\frac{V_2}{F_0} = \frac{x_2 - x_1}{(-r)_2}$$

$$\frac{V_3}{F_0} = \int_{x_2}^{x_3} \frac{dx}{(-r)}$$



Consider PFR + CSTR, CSRT + PFR, if the size of reactors are fixed, then a diff. conversion will be obtained depending on which reactor is placed first. If the int. and overall conversion are fixed the individual reactor volumes as well as total reactor vol. will be diff. depending on arrangement.