Prof. Shankar
[illegible]

Advanced Reaction Engineering

Objective: Comprehend logic of decision making for design operation, evaluation of reacting systems

Process Industry

organic chemicals
biochemicals
Inorganic Chemicals
Fermentation products.

Agriculture

Environment

Biology

Medicine

Methodology: Problem Solving will be the vehicle of communication

Philosophy:

Science is about models of reality.

Equipment Choices

Tubular Vessels

stirred Vessels

Fluid Beds

Rotary Kilns

Blast Furnaces

Criteria of Reactor Choice

Quality

Reliability

Safety

Productivity

cost

Task:

Design, operation

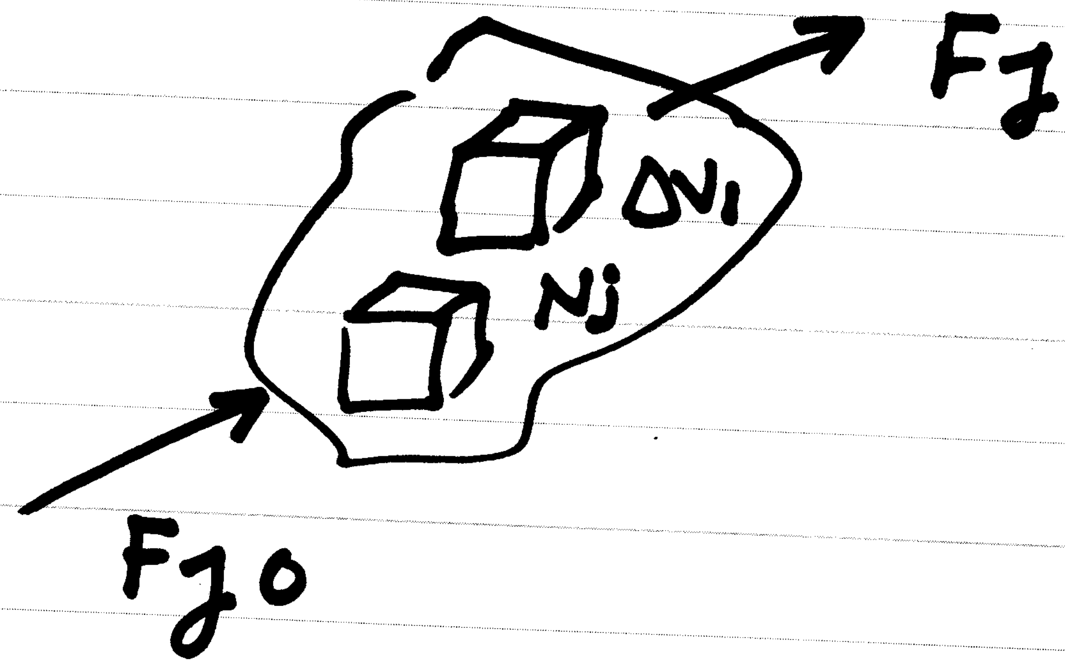
Development

Advanced Reaction Engineering

Design Equations.

DESIGN EQUATIONS

General Balance Equation



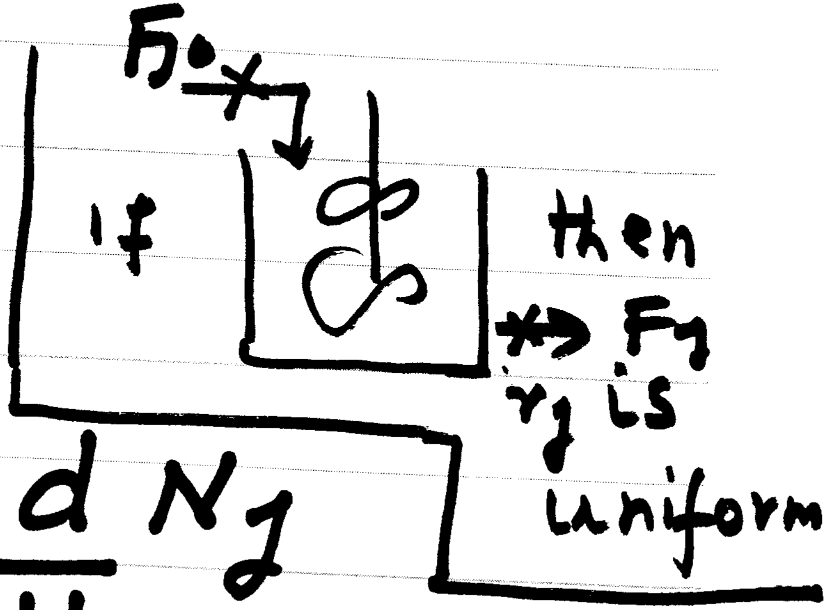
Mole Balance on Species 'j'

$$F_{j0} - F_j + G_j = \frac{d \cdot N_j}{dt}$$

I/P - O/P + Generation = Accumulation

$$G_j = r_{j1}\Delta V_1 + r_{j2}\Delta V_2 + \dots$$

$$= \int_V r_j \, dV$$



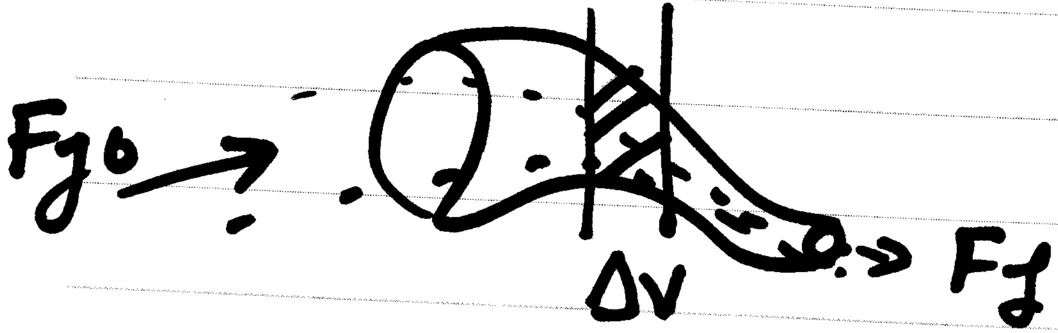
$$F_{j0} - F_j + \int_V r_j \, dV = \frac{d}{dt} N_j$$

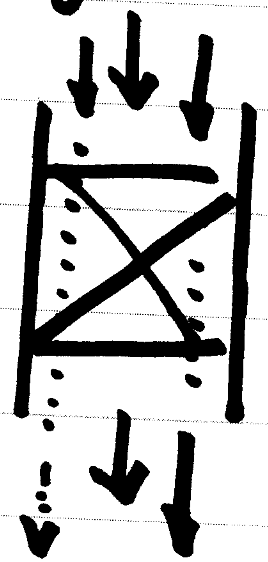
If r_j is uniform over volume V

We have in a stirred vessel

$$F_{j0} - F_j + r_j V = \frac{d}{dt} N_j$$

Balance Equation for Plug flow Vessels





I/P − O/P + Gen = Acc

$$F_j(V,t) - F_j(V+\Delta V,t) + r_j(V,t)\cdot\Delta V = \frac{\partial}{\partial t}(C\,\Delta V)$$

$$\boxed{-\frac{\partial F_j}{\partial V} + r_j = \frac{\partial C_j}{\partial t}}$$

at steady state

$$\frac{\partial F_j}{\partial V} = r_j$$

Plug Flow.

steady state

$$\frac{dF_j}{dV} = r_j$$

Plug flow means fluid elements do not mix as it moves through equipment

stoichiometric Table

$$aA + bB = cC + dD$$

$$A + \frac{b}{a} B = \frac{c}{a} C + \frac{d}{a} D$$

also

$$\frac{r_A}{-a} = \frac{r_B}{-b} = \frac{r_c}{c} = \frac{r_d}{d} = r_1$$

Conversion $X_A = \frac{N_{A0} - N_A}{N_{A0}}$ (Batch Process)

$$X_A = \frac{F_{A0} - F_A}{F_{A0}}$$ ((Continuous)

BATCH SYSTEM $\quad A + \frac{b}{a}B = \frac{c}{a}C + \frac{d}{a}D.$

Species	Moles (Initial)	Moles Remaining
A	N_{A0}	$N_A = N_{A0}(1 - X_A)$
B	N_{B0}	$N_B = N_{B0} - N_{A0}X_A(b/a)$
C	N_{C0}	$N_C = N_{C0} + N_{A0}X_A\, c/a$
D	N_{D0}	$N_D = N_{D0} + N_{A0}X_A\, d/a$
I	N_{I0}	$N_I = N_{I0}$
	N_{t0}	$N_t = N_{t0} + N_{A0}\left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)X_A$

$$N_t = N_{t_0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right) N_{A_0} X_A$$

$$\frac{N_t}{N_{t_0}} = \left(1 + y_{A_0} X_A \delta_A\right)$$

Change in moles due to rxn w.r.t A

$$\delta_A = \left(d/a + c/a - \frac{b}{a} - 1\right) \Rightarrow$$

change in moles due to rxn w.r.t A

$$y_{A_0} = \frac{N_{A_0}}{N_{t_0}}$$

When you use B as reference we get

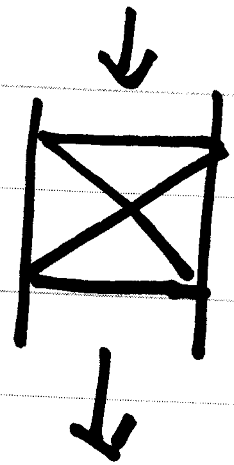
$$\frac{N_t}{N_{t0}} = 1 + y_{B0}\,\delta_B X_B \qquad X_B = \frac{N_{B0} - N_B}{N_{B0}}$$

where $\delta_B = \left(\frac{d}{b} + \frac{c}{b} - a/b - 1\right)$

$$y_{B0} = \frac{N_{B0}}{N_{t0}}$$

FLOW SYSTEM

For a flow system our equations look similar. Simply replace N by F



$$F_t = F_{t0} + F_{A0}(\delta_A) x_A$$

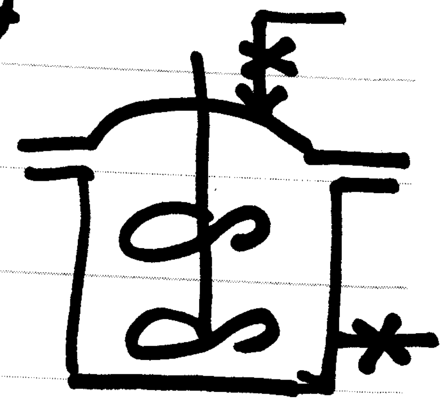
$$\frac{F_t}{F_{t0}} = 1 + y_{A0} x_A \delta_A$$

Design Equation(s) Batch System

Well Stirred Batch

I/p − O/p + Gen = Accumulation

$$\cancel{F_{j0}} - \cancel{F_j} + r_j V = \frac{d}{dt} N_j$$



$$aA + bB = cC + dD$$

$$A + \frac{b}{a} B = \frac{c}{a} C + \frac{d}{a} D$$

$$r_A V = \frac{d}{dt} N_A$$

$$X_A = (N_{A0} - N_A)/N_A$$

$$N_A = N_{A0}(1 - X_A)$$

So $\quad - N_{A0} \dfrac{dX_A}{dt} = r_A V$

$$dt = \frac{N_{A0}\, dX_A}{-r_A V}$$

Integrating

$$t_r = N_{A0} \int_0^x \frac{dX_A}{-r_A \cdot V}$$

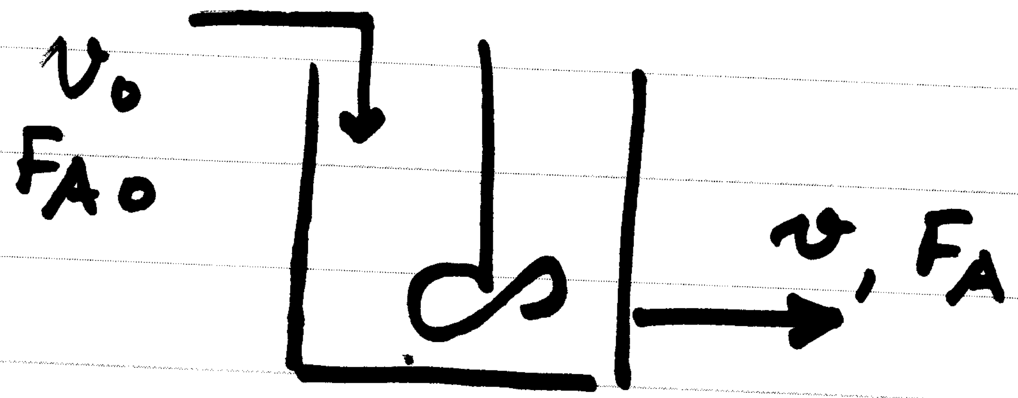
Batch design Eqn

$$t_r = N_{A0} \int \frac{dX_A}{-r_A \cdot V}$$

t_r : Reaction time

Note that if V changes during reaction its effects are taken into account

Design Equation for CSTR (at Steady State)



$$aA + bB = cC + dD$$

$$A = \frac{b}{a}B \pm \frac{c}{a}C + \frac{d}{a}D$$

$$I/p - O/p + Gen = Accumulation$$

$$F_{A0} - F_A + r_A V = \cancel{\frac{dN_A}{dt}}$$

RXN
$aA + bB = cC + dD$

$$F_{A0} X_A = -r_A V$$

$$V = \frac{F_{A0} X_A}{-r_A}$$

$\tau = V/v_0$

Since $V = \dfrac{F_{A0} X_A}{-r_A}$

$$\tau = \frac{C_{A0} X_A}{-r_A}$$

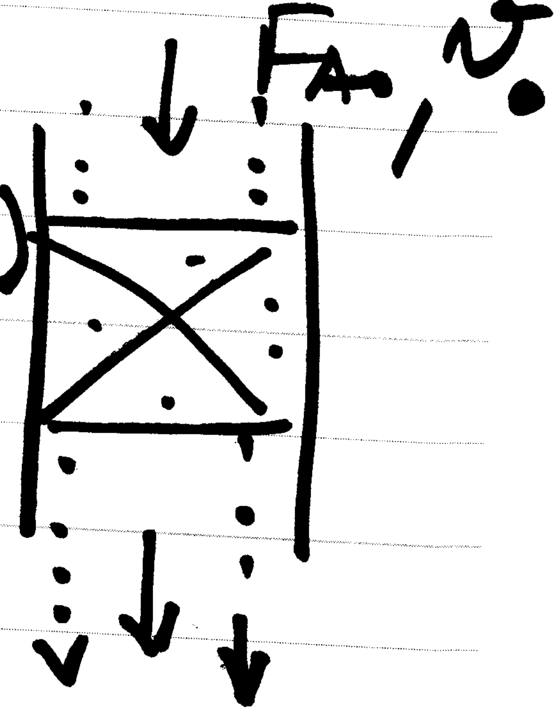
τ: residence time based on inlet flow

PLUG FLOW

$$aA + bB = cC + dD$$

$$\frac{dF_A}{dV} = r_A$$

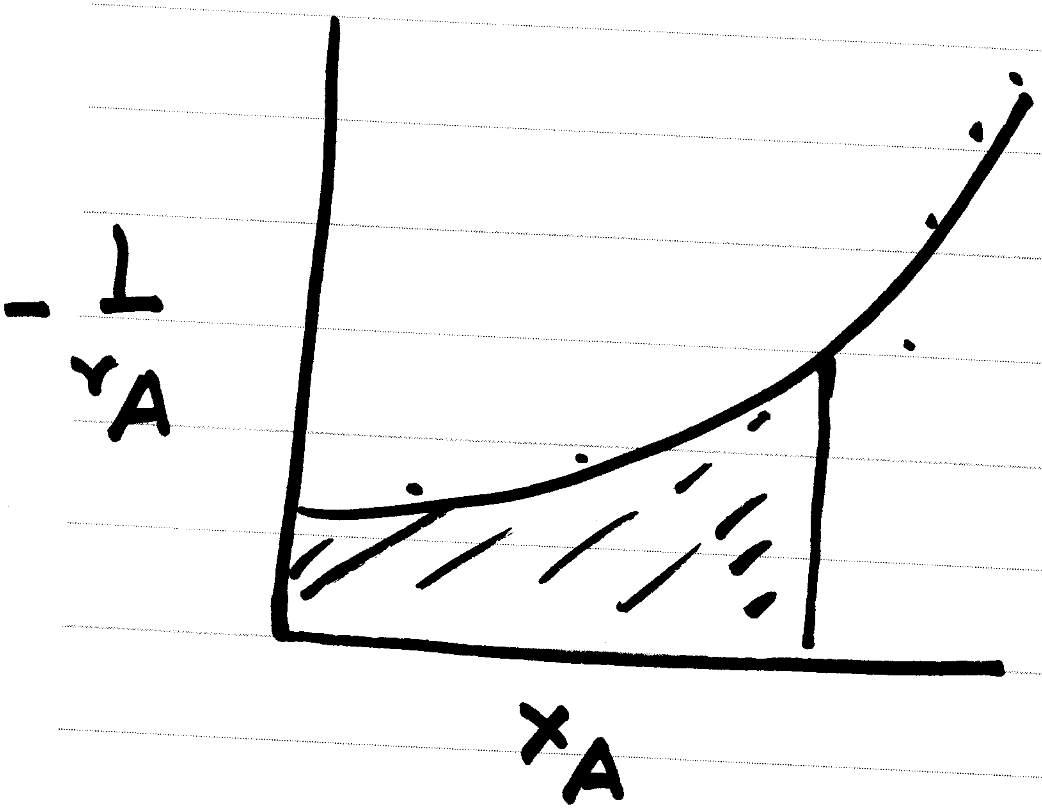
$$F_A = F_{A0}(1 - X_A)$$



$$-F_{A0}\frac{dX_A}{dV} = r_A$$

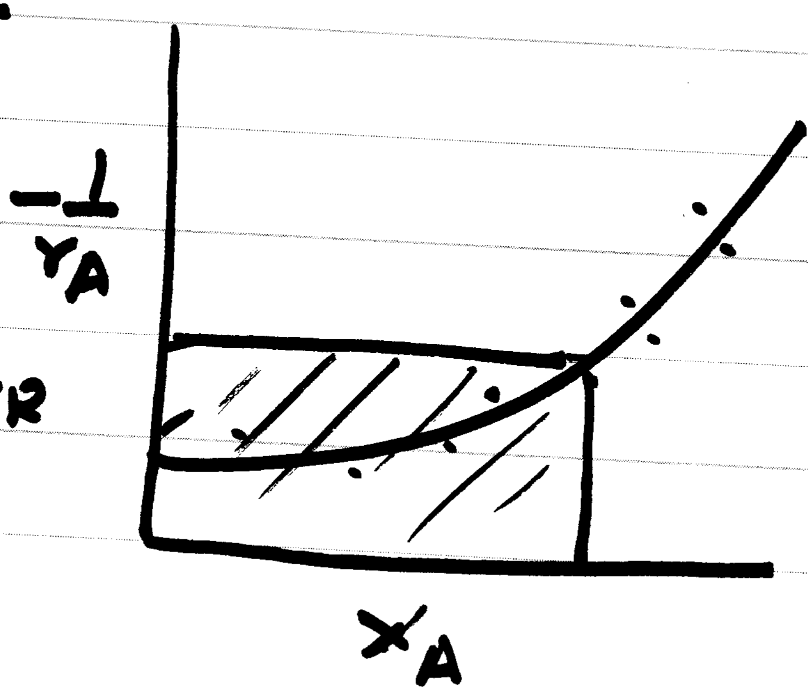
$$V = F_{A0}\int_0^{X_A}\frac{dX_A}{-r_A}$$

$$\tau = V/v_0 = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A}$$



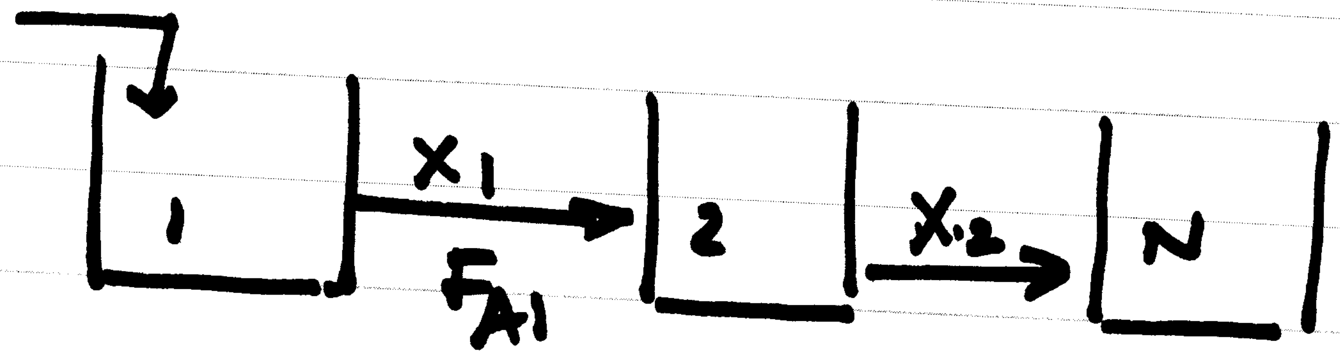
$$V = F_{A0}\int_0^x \frac{dx}{-r_A}$$

PFR



$$V = \frac{F_{A0}\, X_A}{-r_A}$$ single CSTR

Sequence of CSTR's of Equal Volume



$$F_{A0} - F_{A1} + r_{A1} V_1 = 0 \quad \text{Steady state}$$

$$V_1 = F_{A0} X_1 / -r_{A1} \; ; \quad \tau_1 = \frac{C_{A0} X_1}{-r_{A1}}$$

Tank 2

$$F_{A1} - F_{A2} + r_{A2} V_2 = 0$$

$F_{A1} = F_{A0}(1 - X_1)$ by definition

$F_{A2} = F_{A0}(1 - X_2)$ by definition

$$F_{A0}(1 - X_1) - F_{A0}(1 - X_2) + r_{A2} V_2 = 0$$

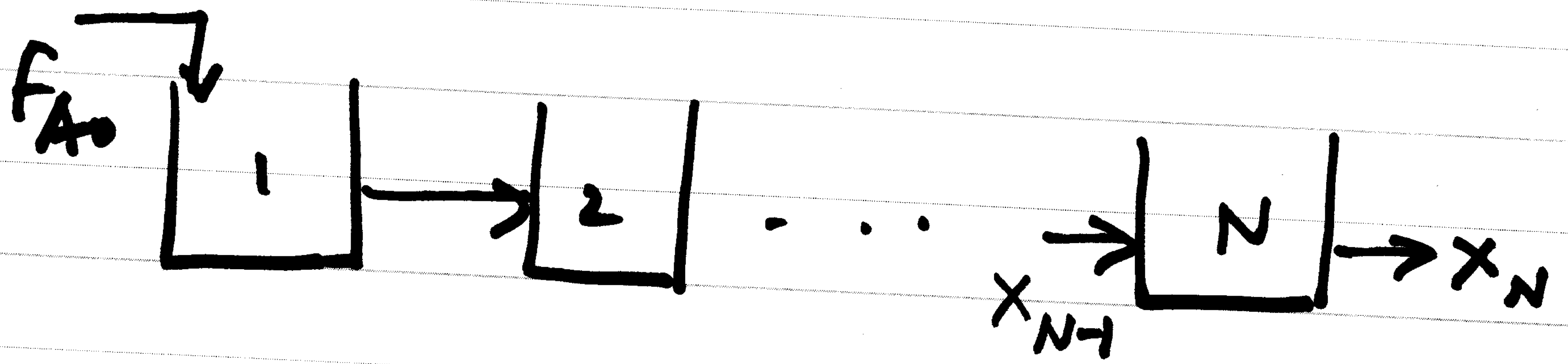
$$F_{A0}(X_2 - X_1) = -r_{A2} V_2$$

$$V_2 = \frac{F_{A0}(X_2 - X_1)}{-r_{A2}} \qquad \tau_2 = V_2 / v_0$$

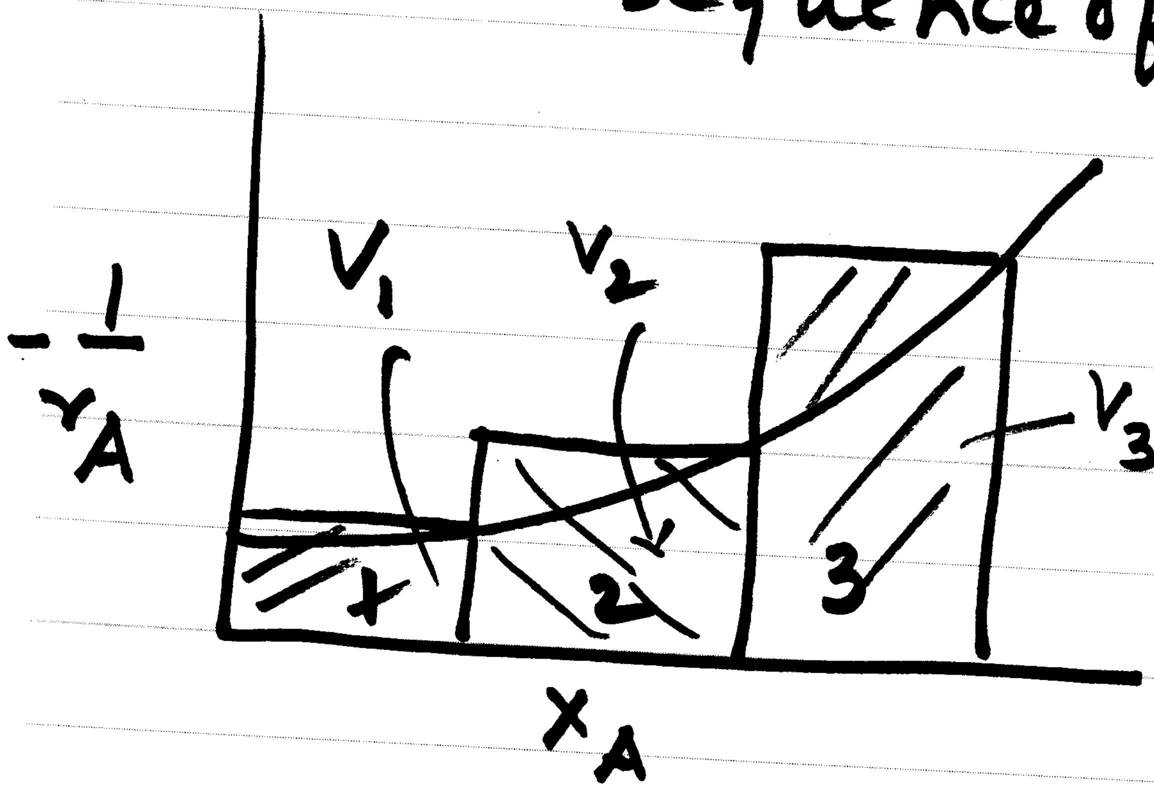
$$\tau_2 = C_{A0}(X_2 - X_1) / (-r_{A2})$$

$$V_n = F_{A0}(X_n - X_{n-1}) / (-r_{An})$$

$$\tau_n = C_{A0}(X_n - X_{n-1}) / (-r_{An})$$



Sequence of CSTRs



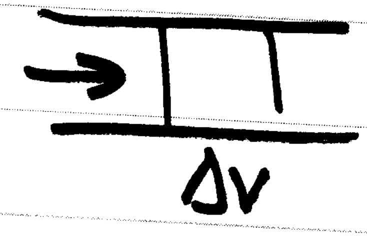
$$aA + bB = cC + dD$$

$$A + \frac{b}{a} B = \frac{c}{a} C + \frac{d}{a} D$$

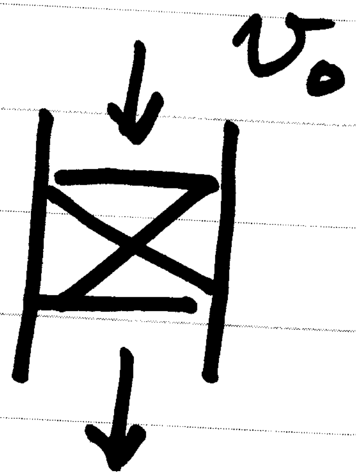
$$V_1 = \frac{F_{A0}(X_1)}{-r_{A1}}$$

$$V_2 = \frac{F_{A0}(X_2 - X_1)}{-r_{A2}} \; ; \quad V_3 = \frac{F_{A0}(X_3 - X_2)}{-r_{A2}}$$

Actual Residence time in PFR



$$aA + bB = cC + dD$$



$$d\tau = dV/v$$

$$\frac{dF_A}{dV} = r_A$$

$$d\tau = \frac{dF_A}{r_A v} = \frac{F_{A0}\, dx_A}{-r_A v}$$

$$\tau = V/v_0$$

$$\tau_{actual} = F_{A0}\int \frac{dx_A}{-r_A v}$$

$$\tau_a =$$

$$\tau_{actual} = F_{A0} \int_0^{X_A} \frac{dX_A}{-r_A \cdot v}$$

volume change occurs due to Stoichiometry of reaction, temperature effects, due to pressure drop.