Reactor design of single reaction

28/08/17

1) Batch Reactors
2) Flow Reactors
3) Multiple reactors connected in series or parallel
4) Reactors with inter stage feed injection or heating
5) Recycling of products to the reactor.

parameters for reactor selection

i) cost of reactor
ii) capacity of reactor
iii) Time of production
iv) Safety consideration
v) Equipment life

Selection of batch reactor

1) small instrument cost
2) Flexibility of operation
3) It has disadvantages of high labor and handling cost i.e each shut down time of cleaning or charging
4) Poorer quality of product
5) Suitable for small scale operations

The time of batch operation is same as plug flow reactors for $\varepsilon_A = 0$ as

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = N_{A0} \int_0^{X_A} \frac{dX_A}{-r_A V}$$

$$\frac{V}{v_0} = \tau_p = C_{A_0}\int_0^{X_A} \frac{dX_A}{-r_A}$$

To acomplish the same job with low capacity process, same size of plug flow reactor and batch reactor are required. For high capacity, batch reactor needs high operating cost and flow reactors should be best option.

<u>CSTR</u>

$$\frac{V_m}{V_0} = \tau_m = \frac{C_{A_0} X_A}{-r_A}$$

<u>PFR</u>

$$\frac{V_p}{v_0} = \tau_p = C_{A_0}\int_0^{X_A} \frac{dX_A}{-r_A}$$

$$\frac{\tau_m}{\tau_p} = \frac{(\tau C_{A_0}^{n-1})_m}{(\tau C_{A_0}^{n-1})_p} = \frac{\frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}}{\int_0^{X_A} \frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}}$$

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

$$\frac{\tau_m}{\tau_p} = \frac{V_m}{V_p} = \frac{\left(\frac{X_A}{(1-X_A)^n}\right)_m}{\left(-\ln(1-X_A)\right)_p}$$

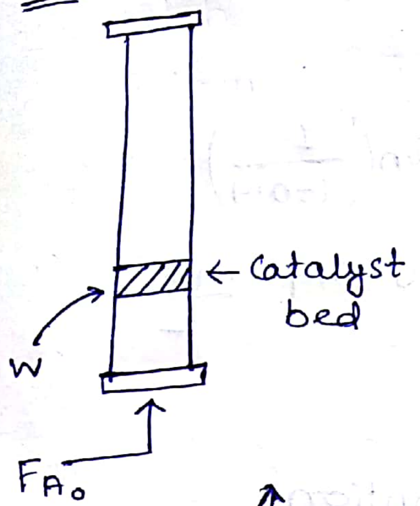
<u>Parameters</u>

1) n
2) X_A
3) ε_A

1) $\frac{V_m}{V_p}$ ↑ with order ↑
2) $\frac{V_m}{V_p}$ depends on ε_A
3) for zero order, independent of type

Tutorial Sheet -3

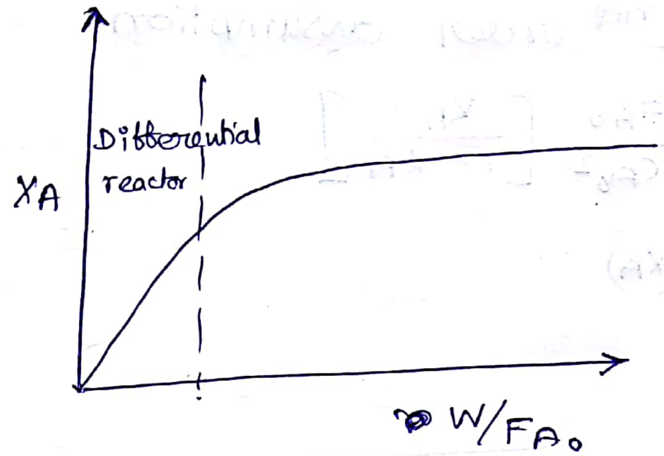
Q.2



$F_{A_0} = 10$ kg mol/hr.

$W =$ variable

$$\frac{dX_A}{d(W/F_{A_0})} = -r_A'$$

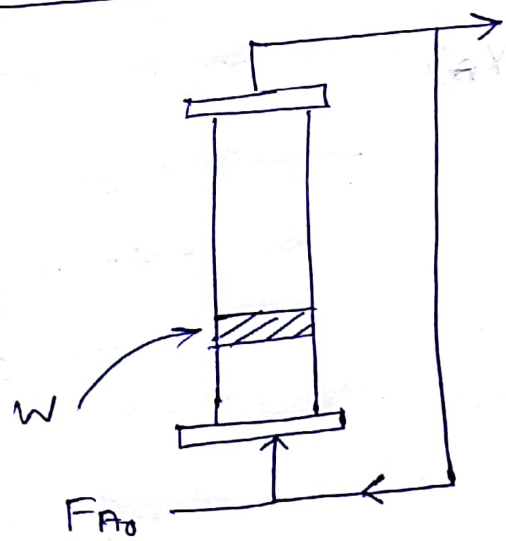


~~Differential reactor~~

a)

b) PFR

c) For very high recycle rate, PFR turns into CSTR.



$$\frac{W}{F_{A_0}} = \int_{X_A=0}^{X_A=f} \frac{dx}{-r_A}$$

by analytical method

$$\frac{W}{F_{A0}} = \frac{1}{kC_{A0}} \int_0^{X_A} \frac{dX_A}{1-X_A}$$

$$Wk = \frac{F_{A0}}{C_{A0}} \ln\left(\frac{1}{1-X_A}\right) = \frac{10}{C_{A0}} \ln\left(\frac{1}{1-0.4}\right)$$

at 1atm & 273°C $\quad C_{A0} = 0.044 \ \frac{mol}{L}$

$$Wk = \frac{10}{0.}$$

From 2^{nd} order assumption

$$Wk = \frac{F_{A0}}{C_{A0}^2}\left[\frac{X_A}{1-X_A}\right]$$

$$= f(X_A)$$

3

Basket reactor at higher rotation speed

$\Downarrow$

CSTR

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

$$C_A = C_{A0}(1-X_A)$$

Optimum Reactor Size

04/09/17

e.g. $A \longrightarrow R \qquad -r_A = kC_A$

$$C_T = \text{total cost} = V \cdot C_M + F_{A_0} C_R$$

Find the optimum cost for a desired capacity

$F_R \ \frac{\text{kmol}}{\text{hr.}}$

C_R = cost of reactant in Rs/Kmol of A

C_M = f (Reactor size)

= ~~Co~~ + cost of installation + overall cost + labour cost } in Rs/hr. (litre of reactant volume)

$$F_R = \text{rate of production of } R$$

$$= F_{A_0} \cdot X_A$$

$$C_T = V \cdot C_M + \frac{F_R}{X_A} C_R$$

For CSTR $\quad V = F_{A_0} \frac{X_A}{-r_A} = \frac{R_{A_0} X_A}{kC_{A_0}(1-X_A)}$

$$V = \frac{F_R X_A}{kC_{A_0}(1-X_A) X_A}$$

$\cancel{C_T = \alpha\left(\frac{1}{X-A}\right) + \frac{\beta}{\beta X_A}}$ $\quad C_T = \frac{F_R C_M}{kC_{A_0}(1-X_A)} + \frac{F_R C_R}{X_A}$

$$C_T = \alpha \frac{1}{(1-X_A)} + \beta \frac{1}{X_A}$$

$$\frac{dC_T}{dX_A} = 0 = \alpha(1-X_A)^{-2} - \beta X_A^{-2} = 0$$

$$V_{opt} = \frac{F_{A_0} X_{Ai,opt}}{kC_{A_0}(1-X_{A,opt})}$$

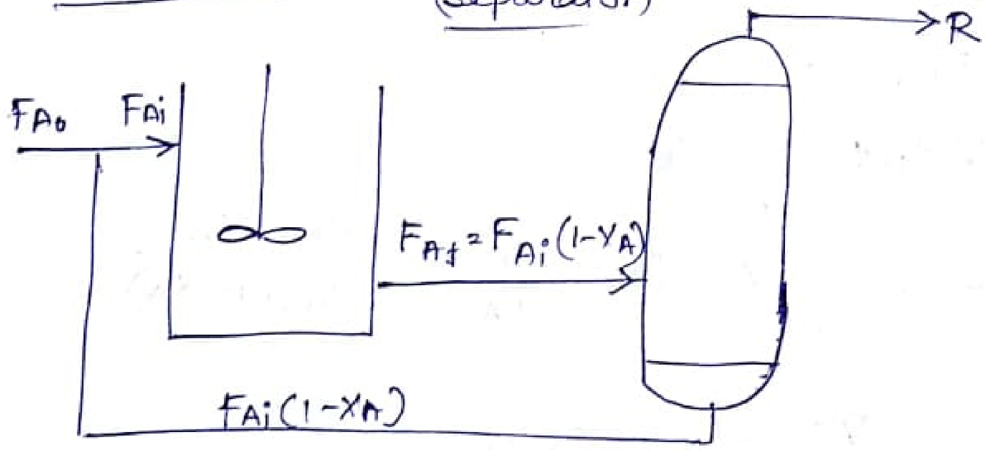
$$\text{Cost of product} = \frac{C_T}{F_R}$$

$$= \frac{V_{opt} C_M + F_{A_0} C_R}{F_R} = \frac{Rs/hr.}{kmol/hr} = \frac{Rs}{kmol}$$

PFR

$$\frac{V}{F_{A_0}} = \int_0^{y_A} \frac{dX_A}{kC_{A_0}(1-X_A)}$$

CSTR with Purification (separator) arrangement



Recycled A

Eg: Optimum Reactor size with Reclaiming unit

$$C_T = V_R C_M + F_{A_0} C_R + F_{Ai}(1-X_A) C_S$$

C_S = unit cost of separation of A

$$F_{Ai}(1-X_A) + F_{A0} = F_{Ai}$$

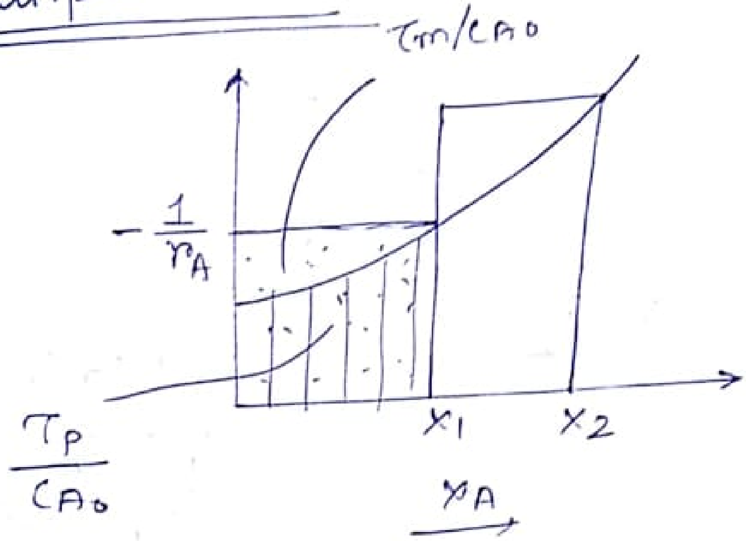
$$F_{Ai} = \frac{F_{A0}}{X_A}$$

$$V_R = \frac{F_{Ai}\, X_A}{K C_{A0}(1-X_A)} = \frac{F_{A0}}{K C_{A0}(1-X_A)}$$

$$C_T = \frac{F_{A0}}{K C_{A0}(1-X_A)} C_M + F_{A0} C_R + \left(\frac{1-X_A}{X_A}\right) F_{A0} C_S$$

Find $X_{optimum}$

Multiple Reactor



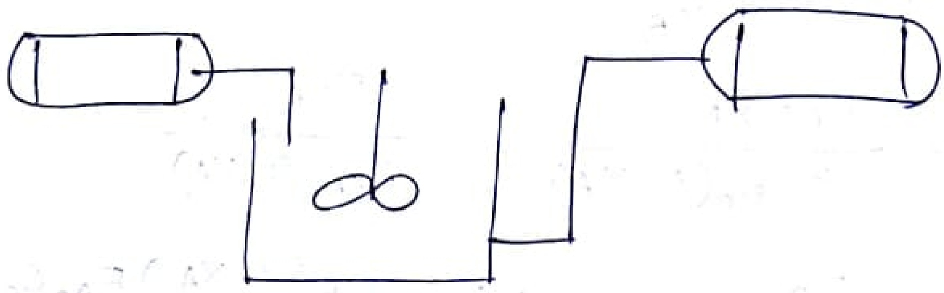
Series reactors

$$\frac{V}{F_0} = \sum_{i=1}^{N} \frac{V_i}{F_0} = \frac{V_1 + V_2 + V_3 + \cdots + V_N}{F_0}$$

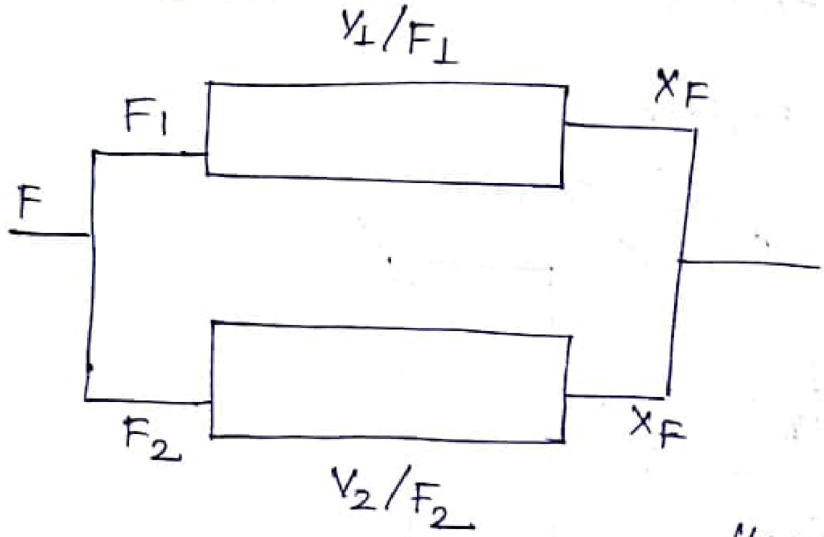
$$\frac{V}{F_0} = \int_0^{X_{A1}} \frac{dX_A}{-r_A} + \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{-r_A} + \cdots + \int_{X_{N-1}}^{X_N} \frac{dX_A}{-r_A} = \int_0^{X_{A1}} \frac{dX_A}{-r_A}$$

So, the conversion obtained in N-PFR in series
= conversion obtained in a single reactor of size, V
$= V_1 + V_2 + V_3 + \cdots + V_N$

e.g



Parallel Reactors



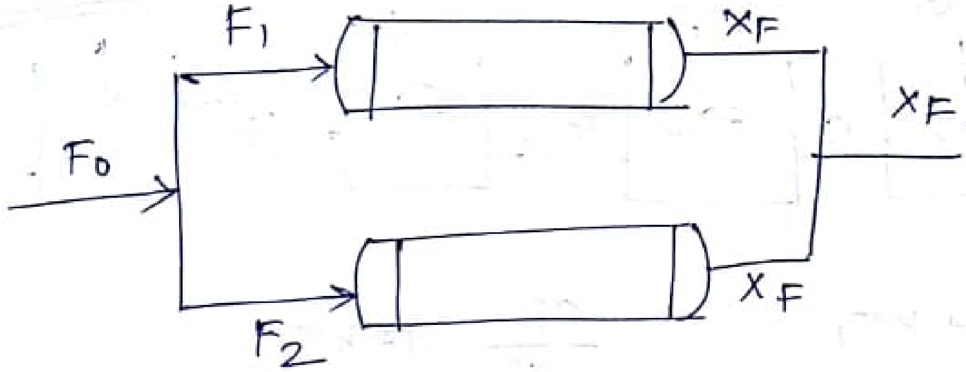
$$\frac{V_1}{F_1} = \frac{V_2}{F_2}$$

Used to increase capacity but not to improve conversion

if $\frac{V_1}{V_2} = 2$, then $F_1/F_2 = 2$ should be kept.

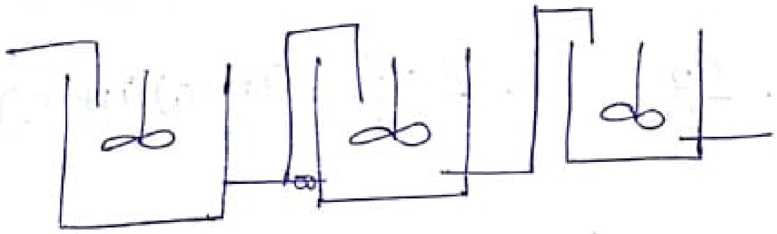
$\frac{V}{F}$ or τ should be kept same. So, the final conversion at the reactor outlet remains same.

Volume of reactor 'V' will vary as 'v_0' changes



$$\frac{V}{F_1} = \frac{X_F}{-r_A}$$

CSTR in series



For i^{th} reactor

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

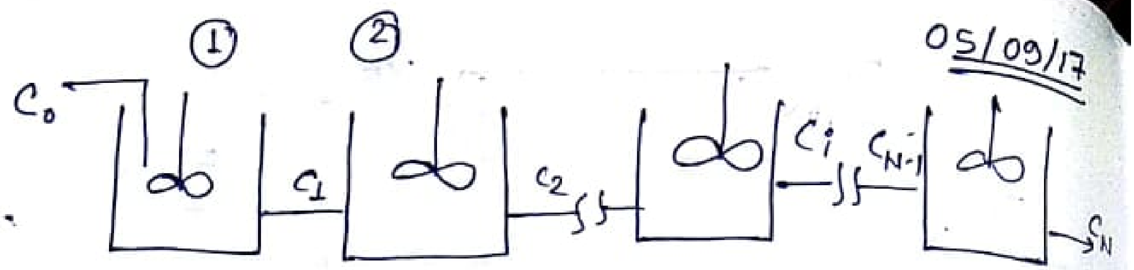
$$\tau_i = \frac{C_0 \left[\left(1 - \frac{C_i}{C_0}\right) - \left(1 - \frac{C_{i-1}}{C_0}\right)\right]}{-r_A} = \frac{C_{i-1} - C_i}{k C_i}$$

$$k\tau = \frac{C_{A0} X_A}{C_{A0}(1 - X_A)} = \frac{X_A}{1 - X_A}$$, . . in general for single ~~se~~ CSTR

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

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

05/09/17



$$\frac{C_0}{C_1} = 1 + k\tau_1 \qquad \frac{C_{i-1}}{C_i} = 1 + k\tau_i$$

$$\frac{C_1}{C_2} = 1 + k\tau_2$$

$$\frac{C_{N-1}}{C_N} = 1 + k\tau_N$$

Assumptions
i) First order
ii) Const. density
iii) Isothermal

$$\frac{C_0}{C_N} = \frac{C_0}{C_1} \cdot \frac{C_1}{C_2} \cdot \frac{C_2}{C_3} \cdots \frac{C_{N-1}}{C_N} = (1+k\tau_1)(1+k\tau_2)(1+k\tau_3)$$

$$\frac{C_N}{C_0} = \frac{1}{(1+k\tau_1)(1+k\tau_2)\cdots(1+k\tau_N)}$$

$$X = 1 - \frac{C_N}{C_0}$$

$$= 1 - \frac{1}{(1+k\tau_1)(1+k\tau_2)\cdots(1+k\tau_3)}$$

e.g 3 reactors in series: V_1, V_2, V_3 being the volume

Assuming: $\tau_1 = \tau_2 = \tau_3 = \cdots = \tau_N = \tau_i$

$$\boxed{\frac{C_0}{C_N} = (1+k\tau_i)^N}$$

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

$$\boxed{\tau_N = \frac{V_T}{v_0} = n\tau_i}$$

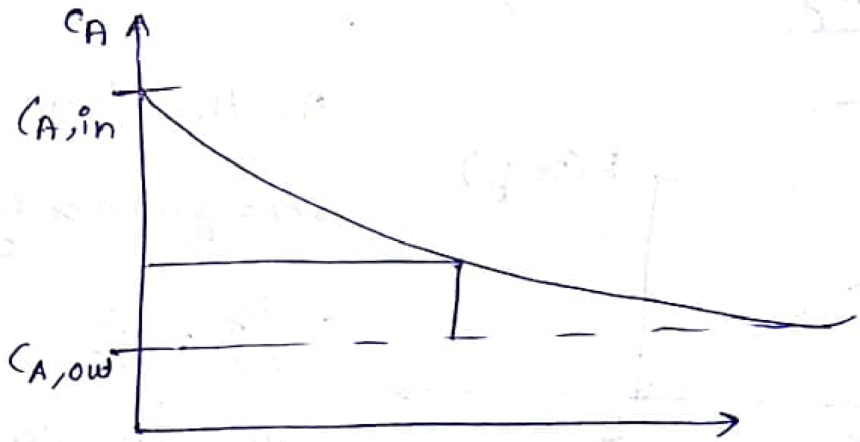
$$\lim_{x\to 0} x\left(y^{1/x} - 1\right) = \ln y$$

$$\tau_N = \frac{N}{K}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right]$$

$$\tau_n = \lim_{N\to\infty} \frac{N}{K}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right]$$

$$\downarrow$$

$$\tau_p = \frac{1}{K}\ln\left(\frac{C_0}{C}\right)$$



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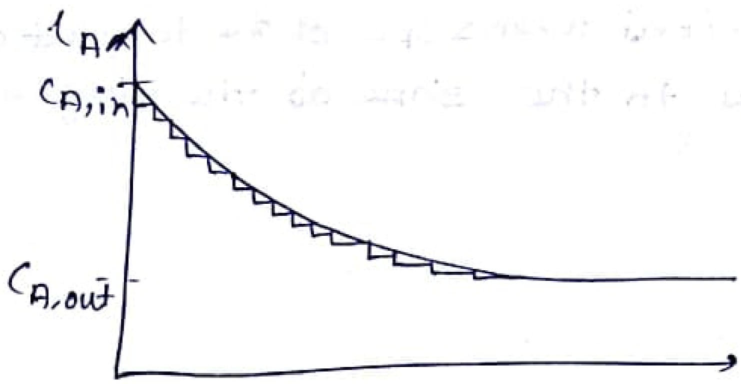


$$\frac{C_0}{C} = (1-x)$$

$$\frac{\tau_N}{\tau_p} = \frac{\frac{N}{k}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right]}{\frac{1}{k}\ln\frac{C_0}{C}}$$

Dam Kohler no.

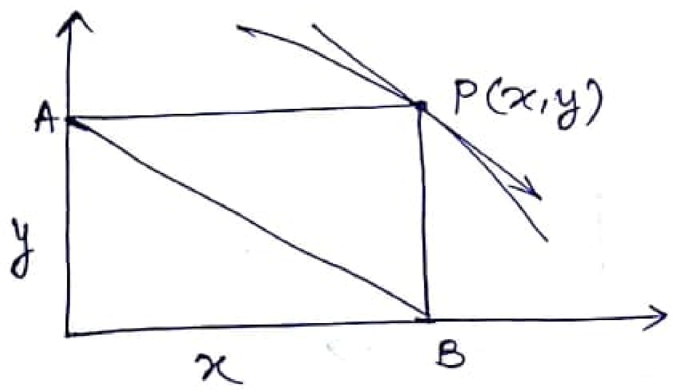
$k\tau \rightarrow 1^{st}$ order

$kC_{A_0}\tau \rightarrow 2^{nd}$ "

$kC_{A_0}^{n-1}\tau \rightarrow$ ~~3rd~~ n^{th} order

Ex. Use of charts for identical mixed reactors
Reber Leveinspiel

Maximizing a Rectangle



A = Area = xy

$dA = y\,dx + x\,dy$

$-\frac{dy}{dx} = \frac{y}{x}$

slope of the diagonal at point P

Area is maximized when slope of the tangent at point P is equal to the slope of the diagonal line AB

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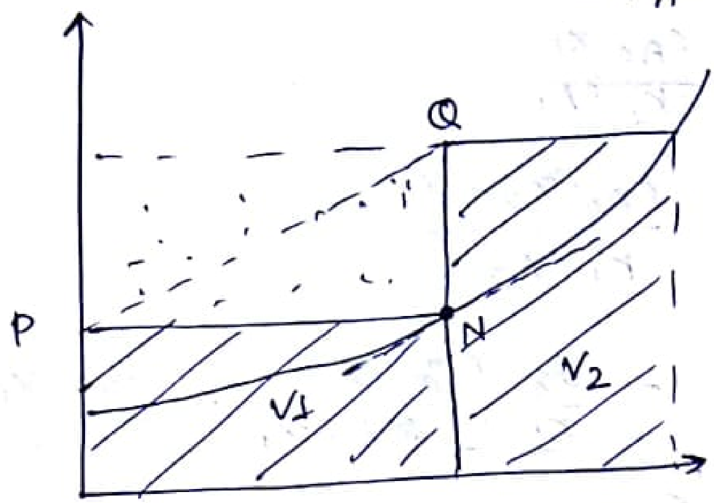
$-r_A = kC_{A_0}(1-X_A)$



$V = V_1 + V_2$

$\frac{dy}{dx} =$ at $x_A = x_1$

$$y = \frac{1}{-r_A} = \frac{1}{kC_{A_0}(1-x_A)}$$

$$\frac{dy}{dx} = \frac{1}{kC_{A_0}(1-x_A)^2}\Big|_{x_A = x_1}$$

$$= \frac{1}{kC_{A_0}(1-x_1)^2}$$

Slope of the diagonal $= \frac{QN}{PN}$

$$= \frac{\frac{1}{kC_{A_0}(1-X_2)} - \frac{1}{kC_{A_0}(1-X_1)}}{x_1}$$

$$x_1 = 1 - (1-x_2)^{1/2}$$

$$V_1 = \frac{v_0}{k}\left(\frac{x_1}{1-x_1}\right) \qquad V_2 = \frac{v_0}{k}\left(\frac{x_2 - x_1}{1-x_2}\right)$$

Fc

Q.17

$$\tau_1 = \frac{V_1}{v_0} = \frac{C_{A0}\, x_1}{k_1\, C_{A1}}$$

$$\tau_2 = \frac{V_2}{v_0} = \frac{C_{A0}(x_2 - x_1)}{k_1\, C_{A2}}$$

De:

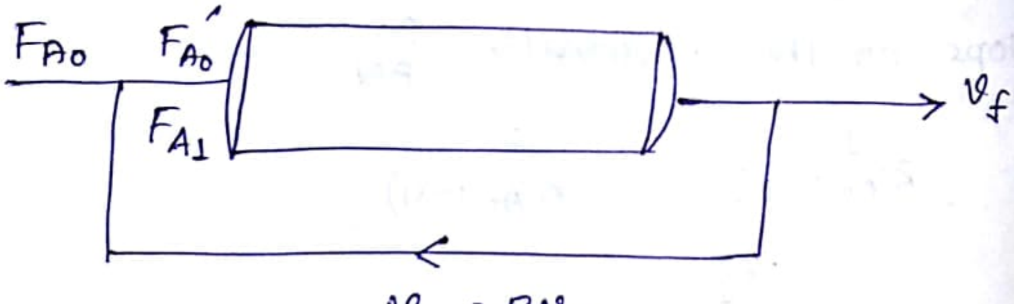
$$V = V_1 + V_2 = \frac{v_0}{k_1}\left[\frac{x_1}{1-x_1} + \frac{x_2 - x_1}{1-x_2}\right]$$

$$\frac{\partial V}{\partial x_1} = \frac{v_0}{k_1}\left[\frac{(1-x_1) - x_1(-1)}{(1-x_1)^2} - \frac{1}{1-x_2}\right] = 0$$

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

11/09/17

Recycle Reactor



$v_3 = R v_f$

R = Recycle ration

$$= \frac{\text{Recycle flow to the feed}}{\text{Product flow rate}} = \frac{v_3}{v_f}$$

$v_3 = R v_f$

R varies

R varies from 0 to ∞

$R \to 0$ It is plug flow reactor

$R \to \infty$ it is mixed flow

$$F_{A0}' = F_{A0} + RF_{A0}$$

$$\frac{V}{F_{A0}'} = \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{-r_A}$$

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

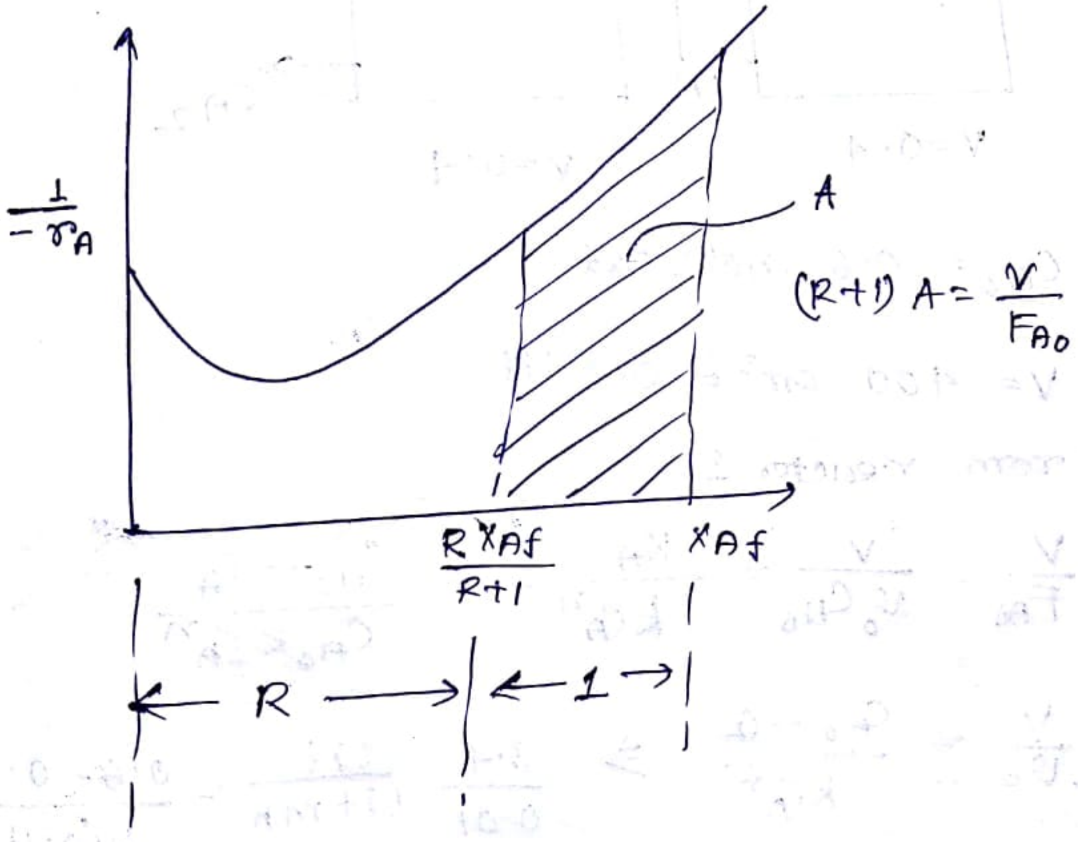
$$A + R \rightarrow R + R$$

$X_{A1} = ?$

$$C_{A1} = \frac{F_{A1}}{v_1} = \frac{F_{A0} + F_{A3}}{v_0 + Rv_f} = \frac{F_{A0} + R\,F_{A0}(1 - X_{Af})}{v_0 + R\,v_0(1 + \epsilon_A X_{Af})}$$

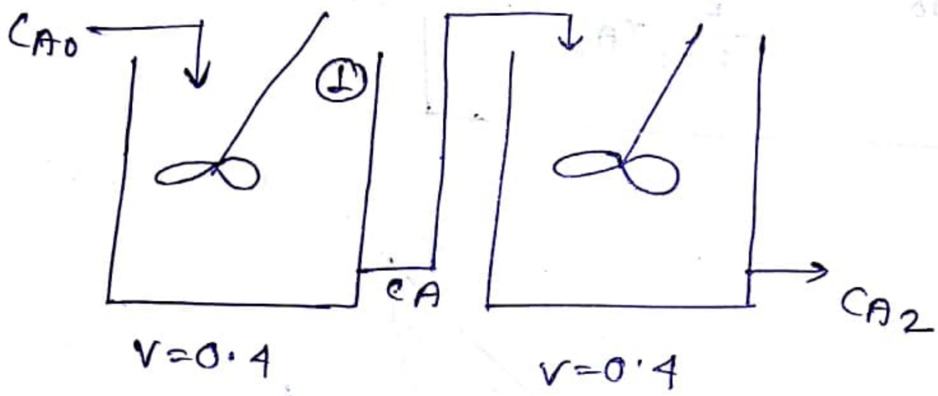
$$C_{A1} = C_{A0}\frac{(1 + R - RX_{Af})}{(1 + R + R\epsilon_A X_{Af})}$$

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



10) Using a color indicator which shows when the concentration of A falls below 0.1 $\frac{mol}{L}$, the following scheme is derived to explore the kinetics of the decomposition of A. A feed of 0.6 mol (A)/Litre is introduced into the first reactor of the of 400 cm^3. The color change occurs in the first reactor for a steady state feed rate of 10 cc/min and in the second reactor for a steady state feed rate of 50 cm^3/min. Find the rate eqn for the decomposition of A from this information.

Sol^n



C_{A_0} = 0.6 moles/cat

V= 400 cm^3 = 0.4 lit

From reactor 1

$$\frac{V}{F_{A0}} = \frac{V}{v_0 C_{A_0}} = \frac{X_A}{k C_A^n} = \frac{C_{A_0} - C_A}{C_{A_0} k C_A^n}$$

$$\frac{V}{v_0} = \frac{C_{A0} - C_A}{k C_A^n} \Rightarrow \frac{0.4}{0.01} \frac{\text{Lit}}{\text{Lit mn}} = \frac{0.6 - 0.1}{k(0.1)^n}$$

$$K(0.1)^n = \frac{0.5}{0.4} \times 0.01 = 0.0125$$

where $v_0 = 50\ cm^3/min$

$$\frac{C_{A2}}{C_{A0}} = \frac{0.6}{0.1} = C_{A1}$$

$$\frac{V}{v_0} = \frac{C_{A1}-C_{A2}}{KC_{A2}^n} = \frac{0.4}{0.05} = 8 \quad \text{--- (2)}$$

$$\frac{V}{v_0} = \frac{C_{A0}-C_{A1}}{KC_A^n} = \frac{0.4}{0.05} = 8 \quad \text{--- (3)}$$

Reactor 2 →

$$\frac{C_A - 0.1}{K(0.1)^n} = 8$$

$$C_{A1} = 8K(0.1)^n + 0.1 = 0.2$$

(3) → $C_{A0} - C_{A1} = 8K\left(C_{A1}\right)^n$

$$K(0.2)^n = 0.05$$

$$n = 2$$

$$K = 1.25$$

$$-r_A = 1.25\, C_A^2 \quad \frac{lit}{mol.\ min}$$

Recycle Reactor

present conversion is $\frac{2}{3}$ for our elementary 2nd order liquid rxn, $2A \rightarrow R$ when operating in an isothermal PFR with a recycle ratio of 1 what will be the conversion if the recycle stream is shut off

Recycle Reactor

$2A \rightarrow 2R$

$-r_A = kC_A^2 \qquad \epsilon = 0$

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

$$k\tau = \frac{2(C_{A0}-C_{Af})}{C_{Af}(C_{A0}+C_{Af})}$$

$$= \frac{2C_{A0}X_A}{C_{A0}(1+X_A)\,C_{A0}(2-X_A)}$$

$C_{A0}k\tau = 2.996$

$$\tau kC_{A0} = \int_0^{X_A} \frac{dX_A}{(1-X_A)^2} \qquad \cancel{R}$$

$$\tau kC_{A0} = 2.996 \simeq 3 = \frac{X_A}{1-X_A}$$

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For recycle reactor 12/09/17

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

$R \to 0$, PFR

$R \to \infty$, CSTR

$$\tau = \frac{C_{A0}V}{F_{A0}} = -(R+1)\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{-r_A}$$

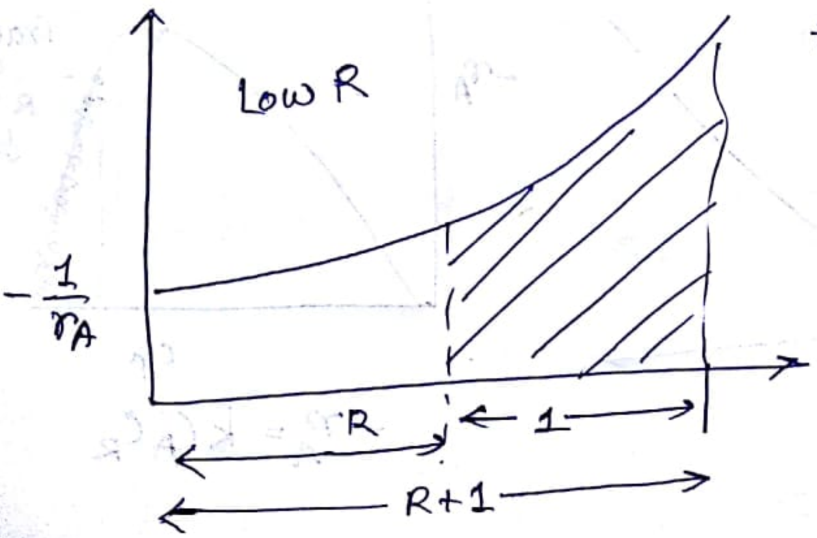
First order

$$-r_A = kC_A \text{ or } -r_A = kC_{A0}(1-X_A)$$

$$\boxed{\frac{k\tau}{R+1} = \ln \frac{C_{A0}+RC_f}{(R+1)C_{Af}}}$$ --- 1st order rxn

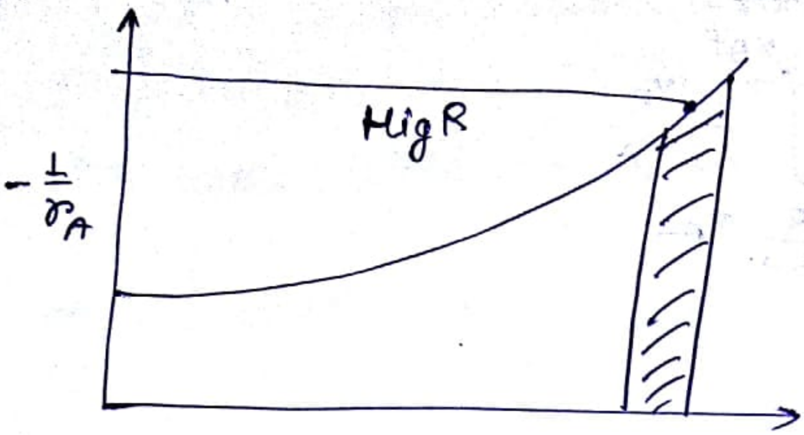
Second-order

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

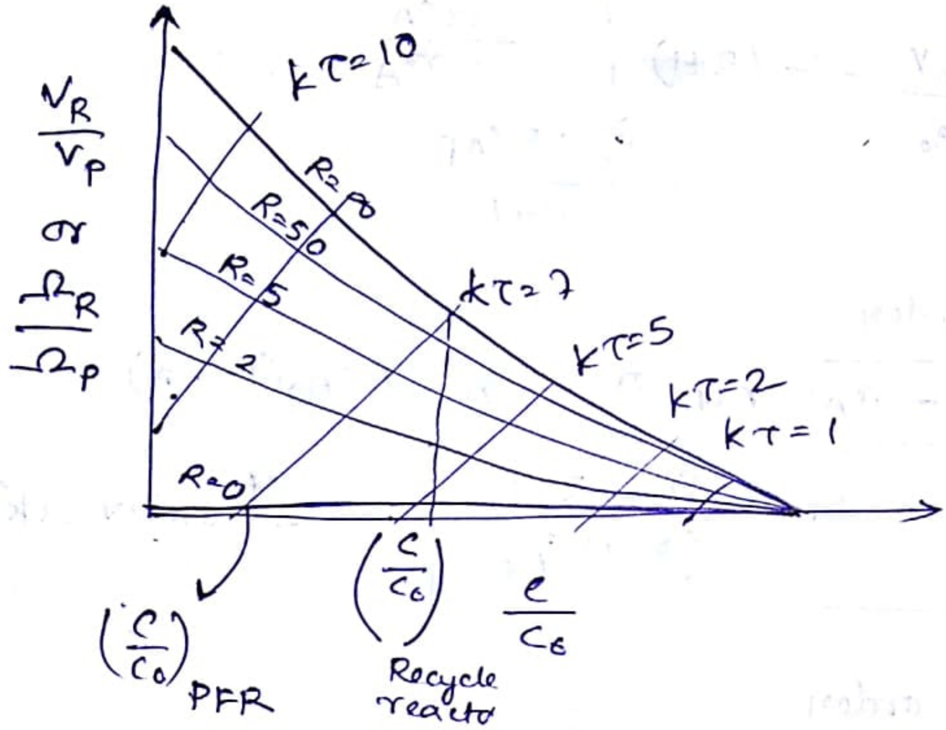


For 1st or 2nd order

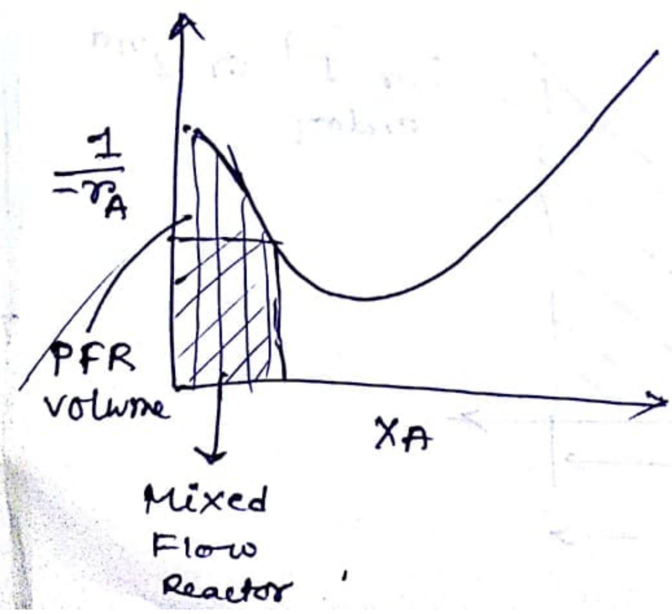
Fo

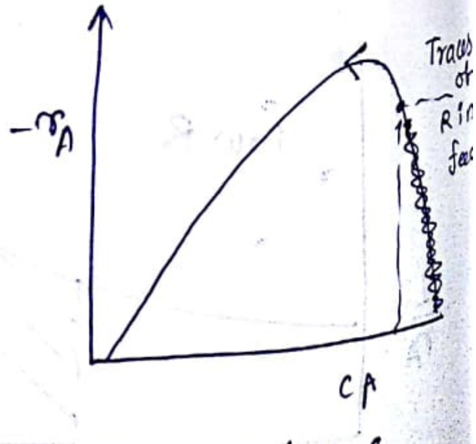


Des



I Auto catalytic reaction





$-r_A = kC_AC_R$

$$\frac{d(\tau/C_{A0})}{dR} = 0$$

From calculus

$$F(R) = \int_{a(R)}^{b(R)} \frac{R+1}{-r_A}\, dX_A$$

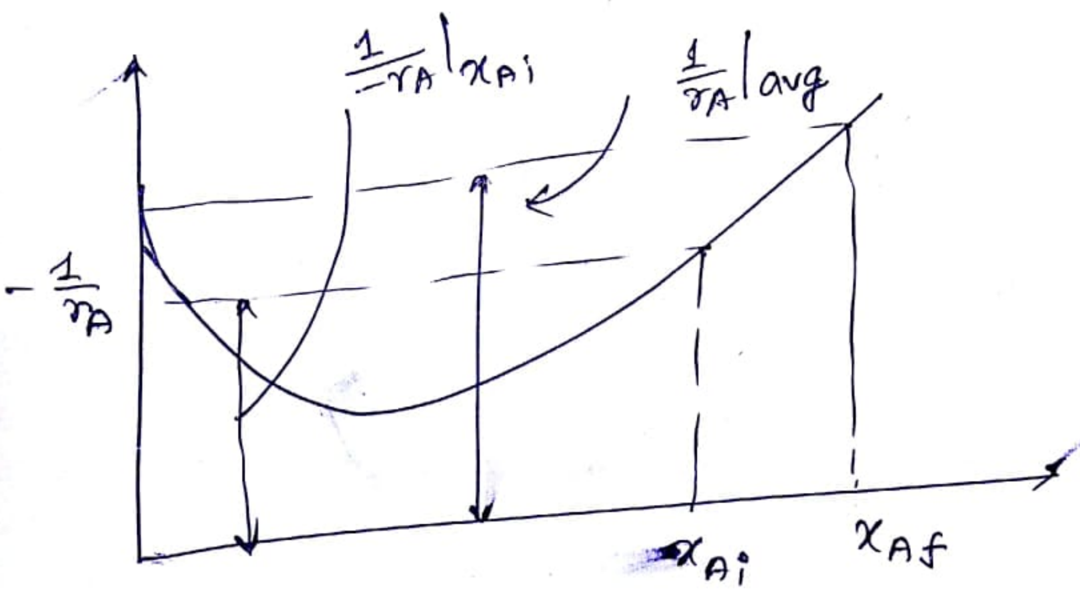
$$\frac{dF}{dR} = \int_{a(R)}^{b(R)} \frac{\partial f(x,R)}{\partial R}\, dx + f(b,R)\frac{db}{dR} - f(a,R)\frac{da}{dR}$$

$b(R) = \text{const.}$ $\frac{db}{dR} = 0$

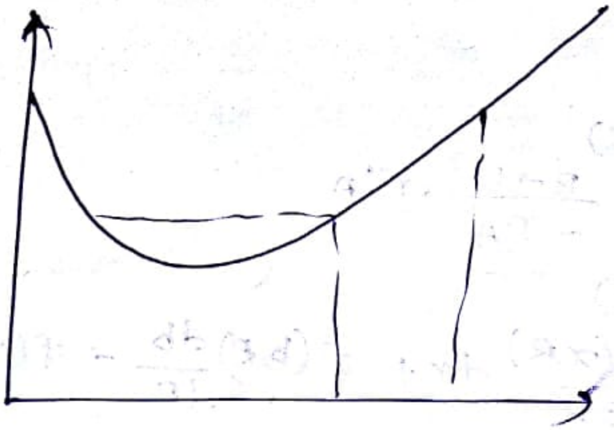
$$a(R) = \frac{R}{R+1} X_{Af} = \frac{X_{Af}}{(R+1)^2}$$

$$f(a,R)\frac{da}{dR} = \frac{1}{-r_A}\bigg|_{x_{Ai}} \left(\frac{X_{Af}}{R+1}\right)$$

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



Fo



$$-\frac{1}{-r_A}\Big|_{avg} = \frac{1}{-r_A}\Big|_{x_{A_f}}$$

Des

(Chapter: 2, 3, 5) Leveinspiel

→ Kinetics derivation, Theories temp. dependance

→ CSTR, Batch reactor, PFR

→ Kinetic study with batch reactor & PFR

Comparison between PFR & CSTR

↓

3 Excercise f^n

$c \rightarrow f(T)$

$P \rightarrow f(T)$

$P_A \rightarrow f(T)$

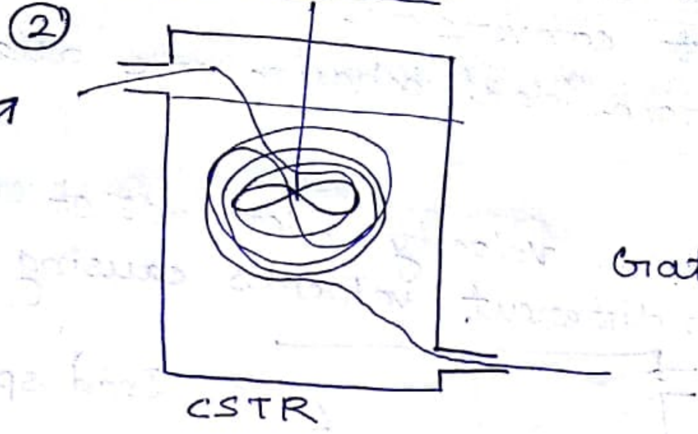
CSTR design

PFR design

I

Residence Time Distribution

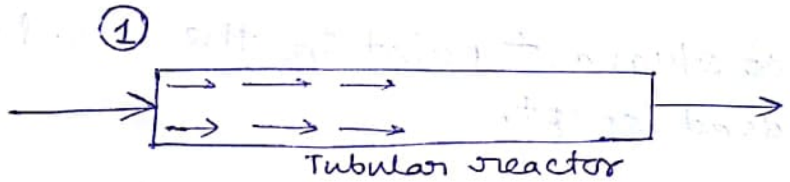
03/10/17



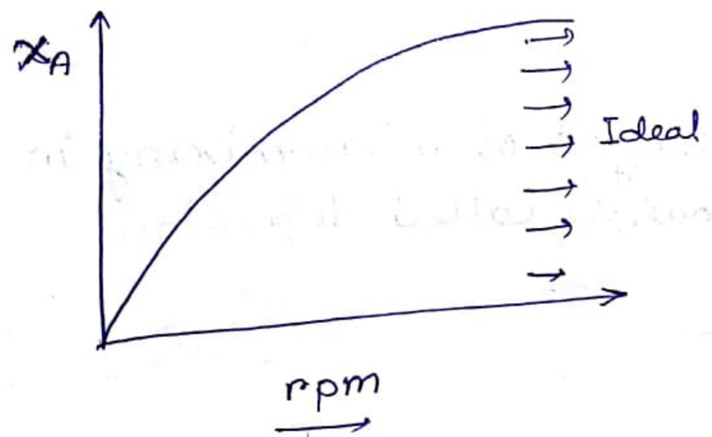
Grates Fault

The ideal behavior in the reaction vessel

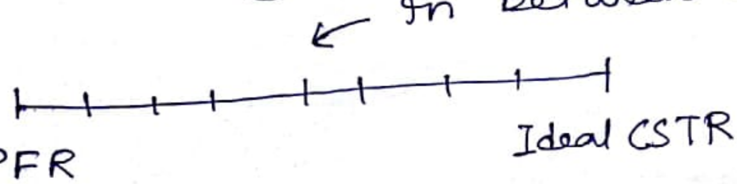
1. Ideal tubular reactor with no axial mixing
2. Ideal stirred tank reactor with complete mixing



If level of micromixing in a reactor is raised then, the tubular reactor converts into CSTR



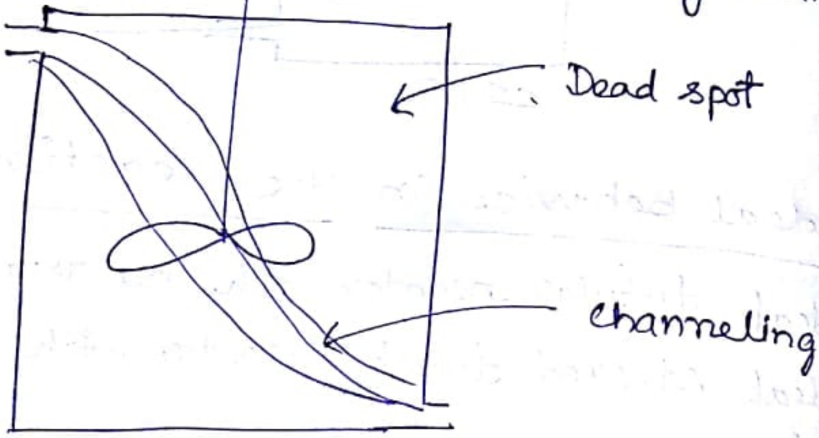
In between stays non-ideal reactor



The extent of non-ideality is important for prediction of conversion

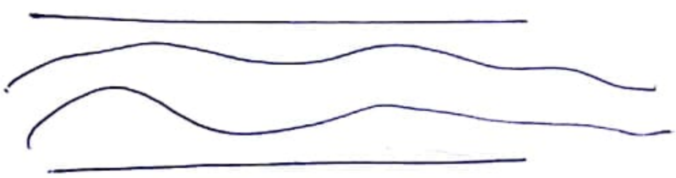
Deviation from ideal behavior are due to following causes

1) Non uniform velocity. Elements of fluid may move with different velocities causing chanelling.



2) Creation of stagnant point in the vessel. It is called dead spot.

Segregation of fluid. (e.g laminar flow)

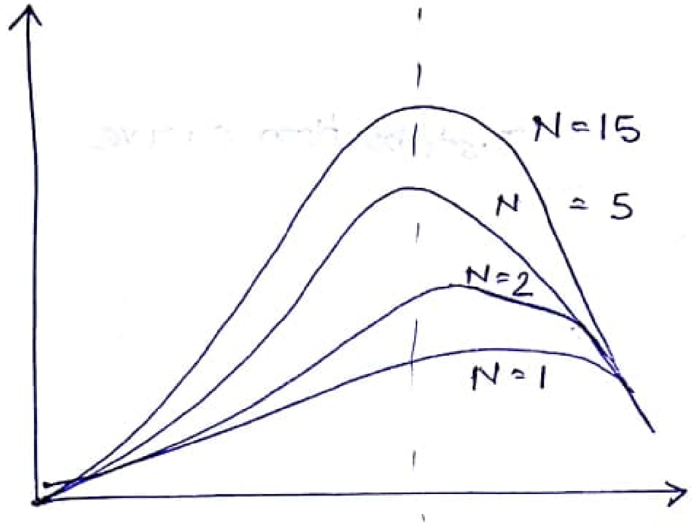


3) Due to development of micro mixing in the direction of flow, it is called dispersion

1) Segregated flow model

2) Equal volume CSTR in series model (N', number is used as parameter)

3) Recycle - Reactor model (Recycle ratio R is the parameter to predict the conversion)

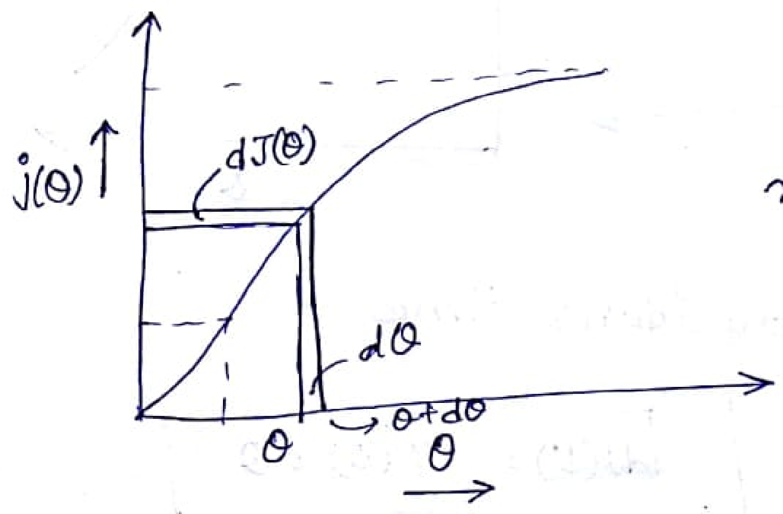


RTD

$$T = \frac{V}{v_0}$$

Average residence time $\equiv$ space time

Let $j(\theta)$ is a fraction of element having residence time less than 'θ' sec.



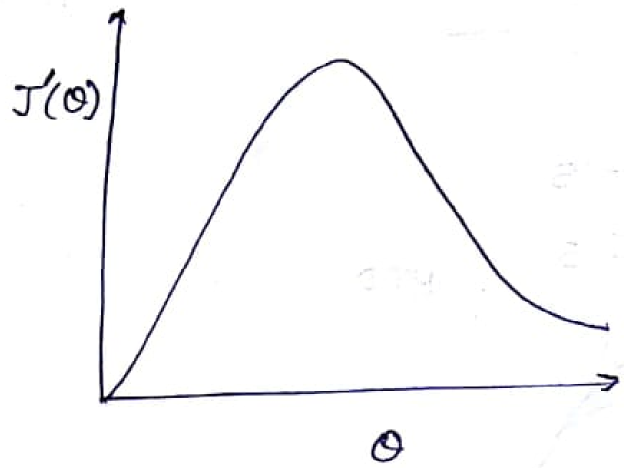
response curve

$J(\theta) = E =$ exit age distribution curve

Fo $\bar{\theta} = \dfrac{\int_0^1 \theta \, dJ(\theta)}{\int_0^1 dJ(\theta)}$ ≡ Average residence time $= \dfrac{V}{v_0}$

* Stimulus response technique

Des



Distribution curve

$F = J'(\theta)$

05/10/17

Two types of functions will be used for RTD analysis

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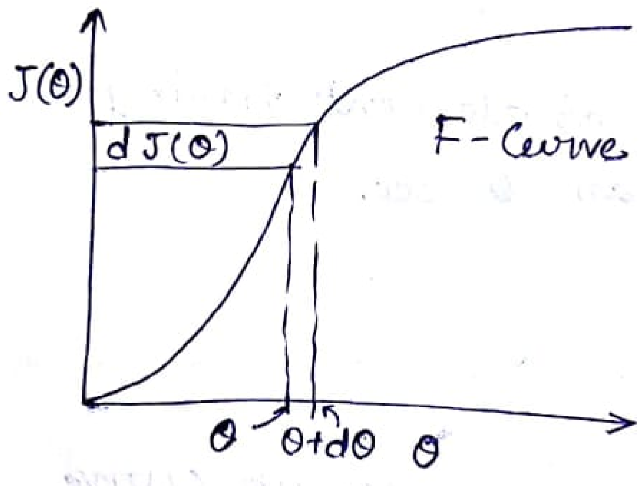
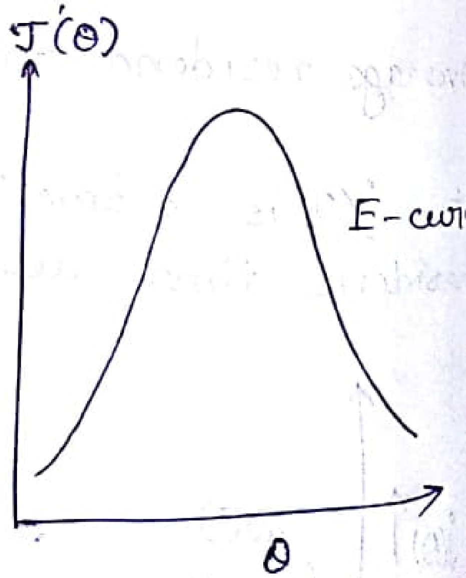


F-Curve



E-curve

$\bar{\theta}$ = Average residence time

$$\boxed{J'(\theta) = \frac{dJ(\theta)}{d\theta}} \qquad \boxed{dJ(\theta) = J'(\theta)\, d\theta}$$

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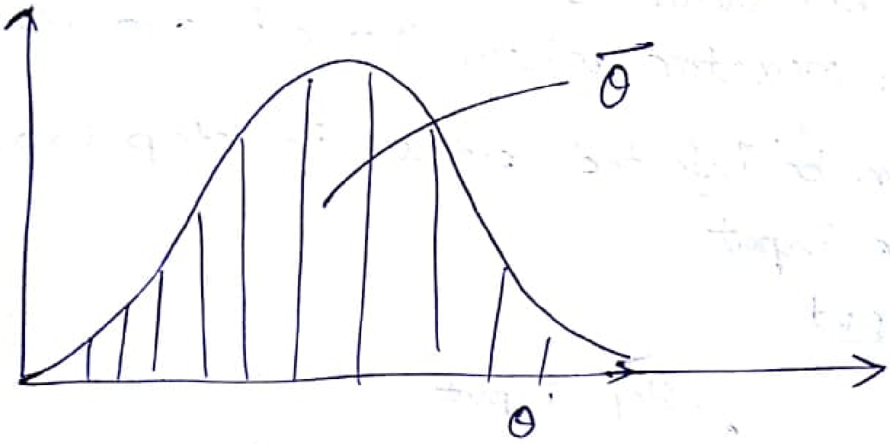
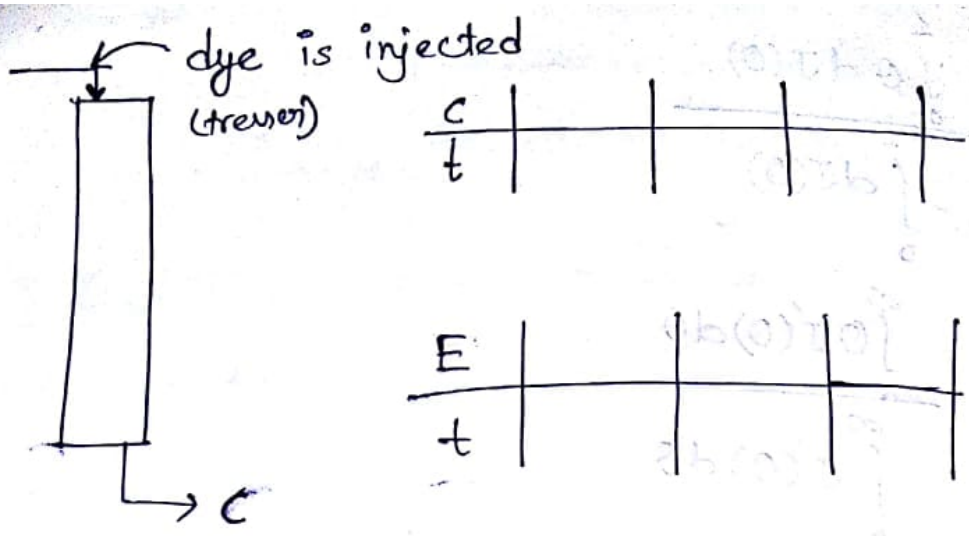
$$\bar{\theta} = \frac{\int_0^1 \theta \, dJ(\theta)}{\int_0^1 dJ(\theta)}$$

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



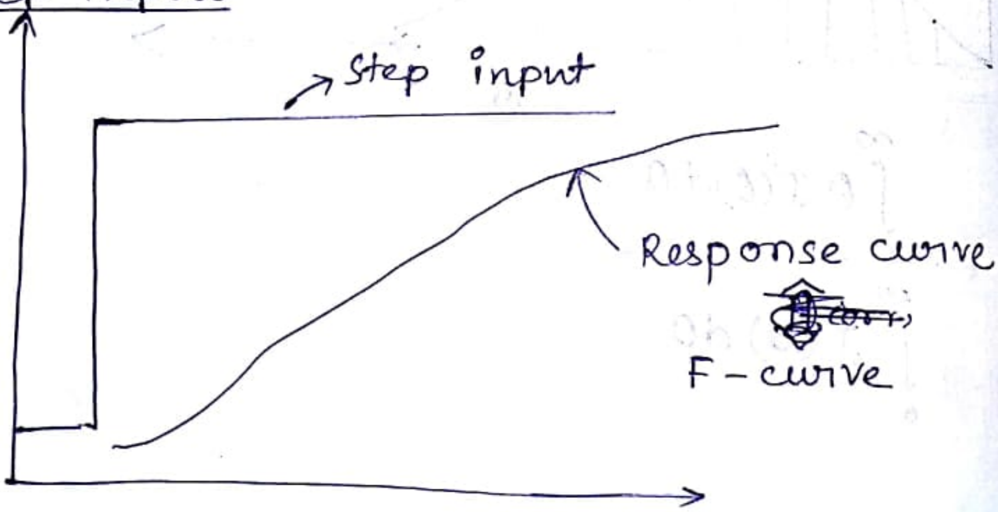
$$\bar{\theta} = \frac{\int_0^\infty \theta J'(\theta) d\theta}{\int_0^\infty J'(\theta) d\theta}$$



* Flow behavior is studied in a ~~vert~~ tubular reactor when there is no reaction

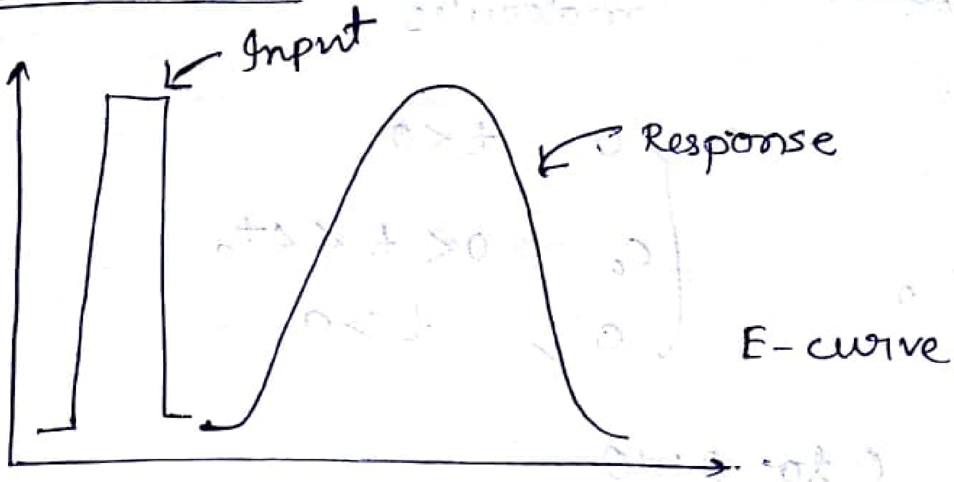
* dye can be injected either in step input or pulse input

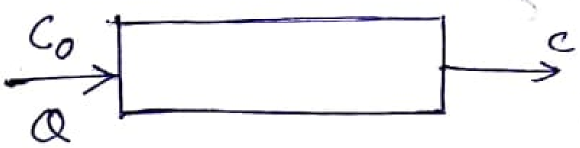
Step input



Step input gives F-curve

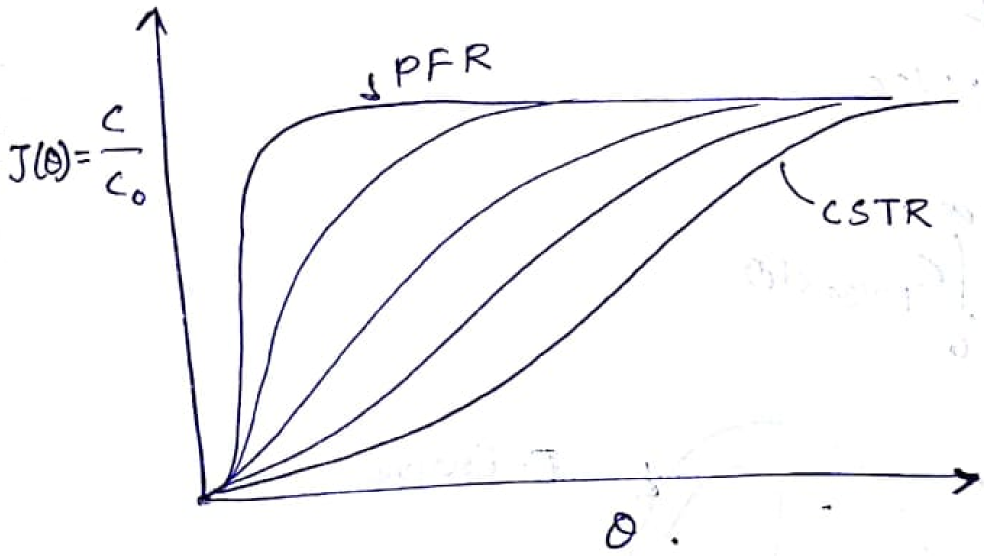
Pulse input





$C_0 Q\, J(\theta) = C \cdot Q$

$J(\theta) = \frac{C}{C_0}$

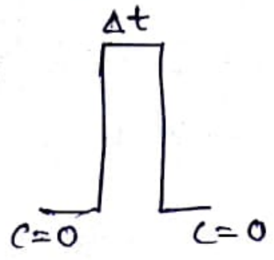


$$\bar{\theta} = \int_0^1 \theta \, dJ(\theta)$$

$$\bar{t} = \int_0^\infty t_i \, E_i \, dt$$

Fc $\quad M = C_0 Q \Delta t \rightarrow$ Total number of marked molecules

Des



$$C = \begin{cases} 0, & t < 0 \\ C_0, & 0 < t < \Delta t_0 \\ 0, & t > 0 \end{cases}$$

Say, for θ to $\theta + d\theta$

No. of molecule leaving $= CQ\,d\theta$

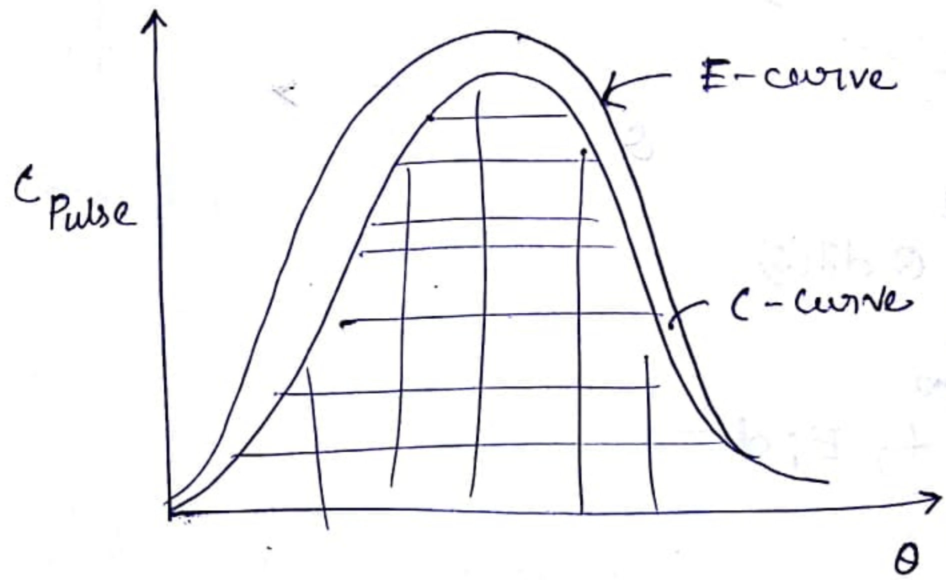
$$\boxed{M J'(\theta)\, d\theta = CQ\, d\theta}$$

$$J'(\theta) = \frac{CQ}{M}$$

C_{pulse}

$$M = Q \int_0^{\infty} C_{pulse}\, d\theta$$

I



$$J'(\theta) = \frac{C_{pulse}\, Q}{Q \int_0^\infty C_{pulse}\, d\theta}$$

$$J'(\theta) = \frac{C}{\int_0^\infty C\, d\theta}$$

$$E \text{ or } J'(\theta) = \frac{C}{\int_0^\infty C\, d\theta}$$

also called normallized concentration

E curve ⇒ Exit age distribution curve

The ~~step~~ relation between step and pulse response

$$J'(\theta)\Big|_{step} = \frac{d\,J(\theta)}{d\theta} = \frac{d\left(\frac{C}{C_0}\right)_{step}}{d\theta}$$

For pulse

$$J'(\theta) = \frac{C_{pulse}\, Q}{M}$$

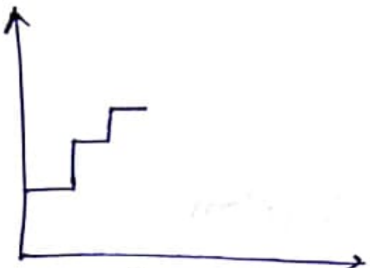
$$C_{pulse} = \frac{M}{Q} J'(\theta) = \frac{(C_0\, Q\, \Delta t_0)}{Q}\, J'(\theta)$$

$$\frac{C_{pulse}}{C_0} = \Delta t_0\, J'(\theta) = \Delta t_0 \frac{d(C/C_0)_{step}}{d\theta} \propto \frac{d}{d\theta}(J(\theta))_{step}$$

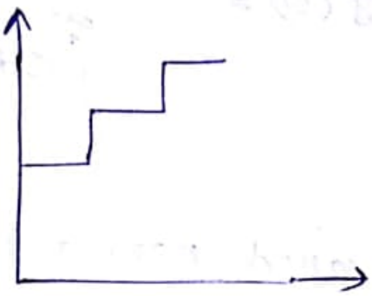
RTD for reactions with known mixing condition

1. Plug Flow
2. Ideal Stirred Tank or mixed reactor
3. Turbulent flow with laminar velocity profile

* In PFR, output profile resembles input profile

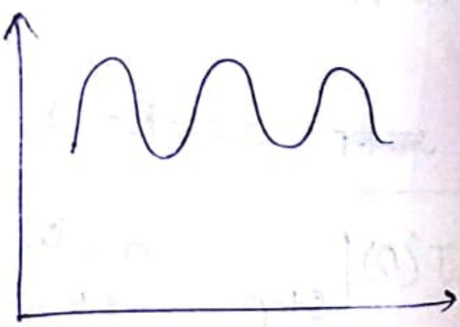


input



output

input



output

$$\frac{V}{F_{A0}} = \int_0^{0.96} \frac{dX_A}{-r_A}$$

$$-r_A = k C_A C_B = k C_{A0} (1-X_A)(C_{B0} - C_{A0}X_A)$$

$$= k C_{A0}^2 (1-X_A)\left(\frac{C_{B0}}{C_{A0}} - X_A\right)$$

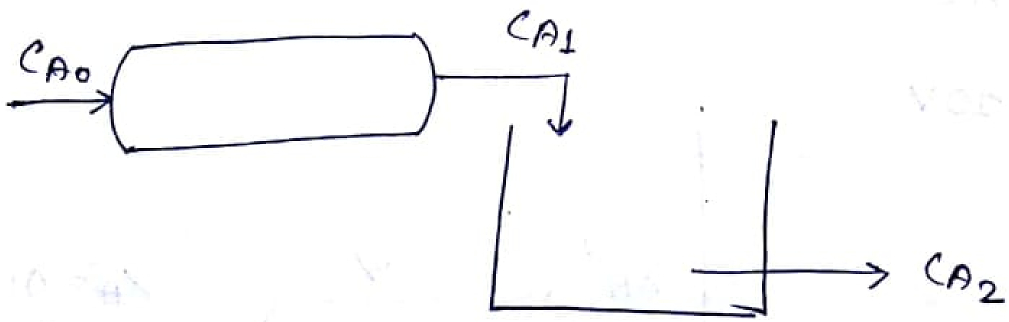
$$= k C_{A0}^2 (1-X_A)^2$$

$$\frac{V}{F_{A0}} = \int_0^{0.96} \frac{dX_A}{k C_{A0}^2 (1-X_A)^2}$$

$$\frac{V}{F_{A0}} = \left[\frac{1}{kC_{A0}^2}\left(\frac{1}{1-x_A}\right)\right]_0^{0.96}$$

$$\frac{VkC_{A0}^2}{F_{A0}} = \frac{1}{0.04} - 1 = 24$$

Option 1



$$\frac{X_{A2}}{C_{A2}} = 0.96$$

$$\frac{V}{F_{A_1}} = \int_0^{x_A'} \frac{d x_A}{k C_{A_0}^2 (1-x_A)^2} \quad \text{---} \ (1)$$

$$\frac{V k C_{A_0}^2}{F_{A_1}} = \left(\frac{1}{1-x_A'} - 1\right)$$

$$\frac{10V}{F_{A_1}} = \frac{0.96 - x_A'}{k C_{A_0}^2 (1-0.96)^2} \quad \text{--} \ (11)$$

$$\frac{V k C_{A_0}^2}{F_{A_0}} = \frac{0.96 - x_A'}{(1-0.96)^2} = 60 - x_A'(62.5)$$

$$x_A' = (60 - 62.5\, x_A')(1 - x_A')$$

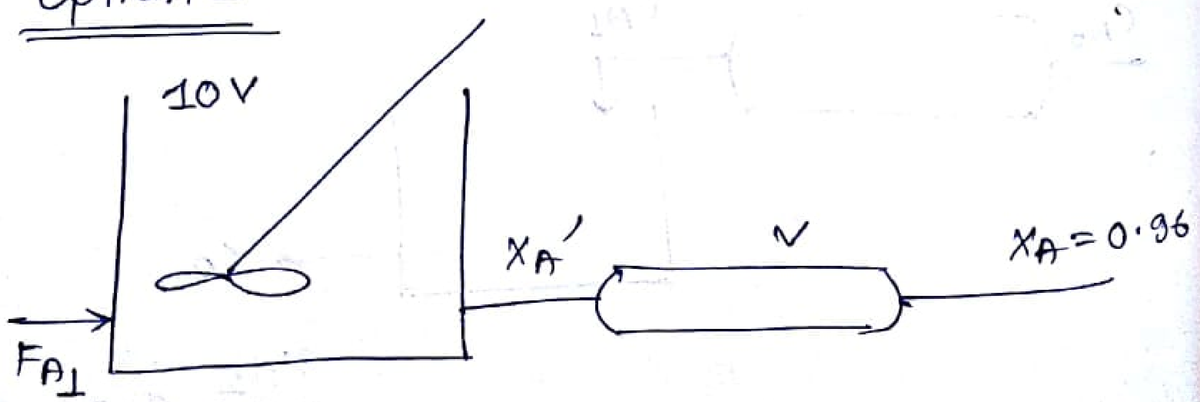
$x_A' = 0.86$ or $x_A' = 1.115$ Rejected)

$$\frac{k C_{A_0}^2 V}{F_{A_0}} = 24, \qquad F_{A_1} = \frac{24}{6.14} F_{A_0}$$

$$x_A' = \frac{123.5 \pm \sqrt{(123.5)^2 - 4(60)(62.5)}}{2 \times 62.5}$$

3.9 times the production increases = $3.9 F_{A_0}$

Option 2



$$\frac{10V}{F_{A1}} = \frac{x_A'}{k\,C_{A0}^2 (1-x_A')^2}$$

$$\frac{V}{F_{A1}} = \int_{x_A}^{0.96} \frac{dx_A}{k\,C_{A0}^2 (1-x_A')^2} = \left[\frac{1}{k\,C_{A0}^2} - \frac{1}{1-x_A}\right]_{x_A'}^{0.96}$$

$$\frac{x_A'}{10(1-x_A')^2} = \frac{0.96-x_A'}{1-0.96}$$

$$10x_A'^2 - 19.64\,x_A' + 9.6 = 0$$

$$x_A' = \underbrace{1.05}_{\text{Rejected.}} \text{ or } 0.916$$

$$\frac{10V\,kC_{A0}^2}{F_{A1}} = \frac{x_A'}{(1-x_A')^2} = 129.82$$

$$F_{A1} = F_{A0}\,\frac{24}{12.982} = 1.849\,F_{A0}$$

First option is applicable

2)

$$C_{A0} x_A = C_{B0} x_B$$

$$-r_A = 5 C_{A0}(1-x_A)(C_{B0} - C_{A0} x_A)$$

$$= 5 C_{A0}^2 (1-x_A)(M - x_A)$$

$$M = \frac{C_{B0}}{C_{A0}}$$

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Sol^n // Problem 2 assignment 4 10/10/17

Basis: 1 hr. operation

$$A + B \longrightarrow R + S$$

Given $-r_A = 5 C_A C_B$ $M = \frac{C_{B_0}}{C_{A_0}}$

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

$$C_{A_0} = 0.1 \text{ mole/L}$$

Mole balance CSTR

$$\frac{V}{v_0} = \frac{C_{A_0} x_A}{-r_A} = \frac{C_{B_0} x_B}{-r_B} \Rightarrow \frac{V}{F_{B_0}} = \frac{x_B}{-r_B}$$

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

$$\boxed{\begin{aligned} C_{A_0} x_A &= C_{B_0} x_B \\ x_B &= \frac{C_{A_0} x_A}{C_{B_0}} \end{aligned}}$$

$$F_{B_0} = \frac{-r_B V}{x_B}$$

$C_T = F_{B_0} \times$ unit price + (Cap cost, Op cost etc.)

$$\boxed{C_T = \frac{56.25 \times 5 C_{A_0} C_{B_0} (1 - x_A)(M - x_A) V}{x_A} + 0.18 V}$$

--- (1)

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$$F_{B_0} = \frac{-r_B V}{x_B} \Rightarrow F_R = F_{A_0} x_A \ , \quad x_A = \frac{F_R}{F_{A_0}} = \frac{95}{1000}$$

$$= 0.95$$

$$\frac{V}{F_{A_0}} = \frac{x_A}{-r_A} , \quad M = \frac{C_{B_0}}{C_{A_0}} = 10\, C_{B_0}$$

$$V = \frac{100\, x_A}{k C_{A_0}^2 (1-x_A)(M-x_A)}$$

$$\boxed{V = \frac{38000}{10\, C_{B_0} - 0.95}} \quad \ldots \ (2)$$

$$C_T = 534375\, C_{B_0} + \frac{6840}{10\, C_{B_0} - 0.95}$$

$$\frac{dC_T}{dC_{B_0}} = 53437.5 - \frac{68400}{(10 C_{B_0} - 0.95)^2} = 0$$

$$C_{B_0} = 0.208 \ \frac{mol}{L}$$

$$C_T = 17168 \text{ Rs.}$$

$$\boxed{V = 33628.3 \ \text{lit}}$$

For PFR

$$C_T = 56.25\, F_{B_0} + 0.68\, V$$

$$V = F_{A_0} \int_0^{0.95} \frac{dx_A}{0.05 (1-x_A)(M-x_A)}$$

$$V = \frac{2000}{(M-1)} \int_0^{0.95} \left[\frac{1}{1-x_A} - \frac{1}{M-x_A}\right] dx_A$$

$$V = \frac{2000}{(M-1)} \ln\left(\frac{M-0.95}{0.05M}\right)$$

$$C_T = 56.25\, M \times 100 + \frac{0.68 \times 2000}{(M-1)} \ln\left(\frac{M-0.95}{0.05M}\right)$$

$$\frac{dC_T}{dM} = 56.25 \times 100 - \frac{0.68 \times 2000}{(M-1)^2} \ln\left(\frac{M-0.95}{0.05M}\right)$$

$$+ \frac{0.68 \times 2000}{(M-1)} \left[\frac{1}{\frac{M-0.95}{0.05M}} \times \frac{(M-0.95)(0.05) - (0.05M)}{(0.05M)^2}\right]$$

$$5625(M-1)^2 + 1292 \frac{(M-1)}{(M-0.95)M} = 1360 \ln \frac{M-0.95}{0.05M}$$

Assumed, M	LHS	RHS
2	6240.2	3197.87
1.5	2189.2	2709.7
1.6	2770.38	2849.12
1.61	2834.75	2861.42
1.615	2867.4	2867.46

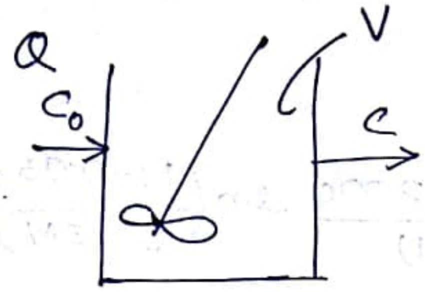
$$M_{optimum} = 1.615 = \frac{F_{B0}}{F_{A0}}$$

$V = 6856.5$ lit

$C_T = ₹13746.85$

Non ideal Reactor

CSTR/ Step input



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

$$\frac{dC}{d\theta} = \frac{Q}{V}(C_0 - C)$$

$$\frac{dC}{d\theta} = \frac{1}{\bar{\theta}}(C_0 - C)$$

$$\int_0^C \frac{dC}{C_0 - C} = \int_0^\theta \frac{d\theta}{\bar{\theta}}$$

$$\left(\frac{C}{C_0}\right)_{step} = J(\theta) = 1 - e^{-\theta/\bar{\theta}}$$

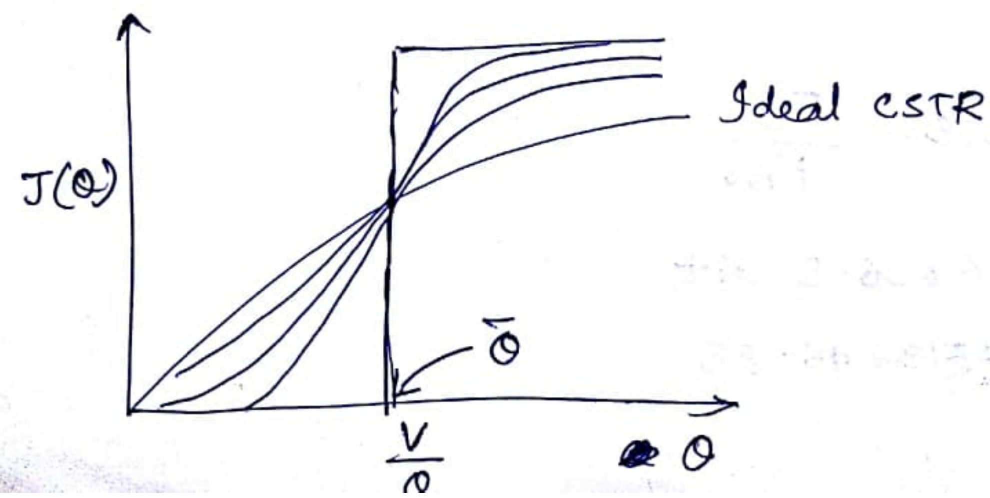
$$F = 1 - e^{-\theta/\bar{\theta}}$$

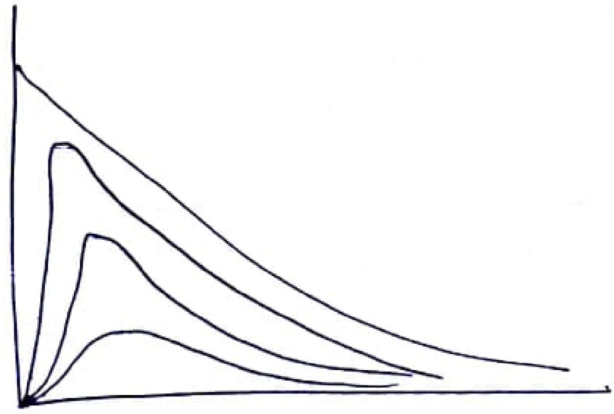
$$E = J'(\theta) = \frac{1}{\bar{\theta}} e^{-\theta/\bar{\theta}}$$

again $\quad C_{pulse} = \frac{M}{Q} J'(\theta)$

$$= \frac{M}{Q} \frac{1}{\bar{\theta}} e^{-\theta/\bar{\theta}}$$

$$C_{pulse} = \frac{C_0 \Delta t_0}{\bar{\theta}} e^{-\theta/\bar{\theta}}$$



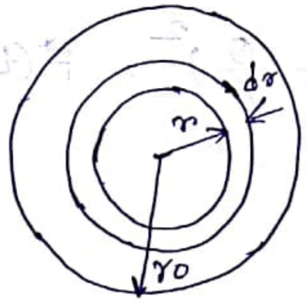


Laminar Flow Model to predict Dispersion

16/10/17

$$u(r) = \frac{2Q}{\pi r_0^2}\left[1 - \left(\frac{r}{r_0}\right)^2\right]$$

r_0 = radius of the tube



$\theta \to \theta + d\theta$, $r \to r + dr$

$$dJ(r) = dJ(\theta) = \frac{u(2\pi r\, dr)}{Q}$$

$$\theta = \frac{L}{u} = \frac{\pi r_0^2}{2Q}\frac{L}{[1-(r/r_0)^2]} = \frac{V/Q}{2\left[1-\left(\frac{r}{r_0}\right)^2\right]}$$

$$= \frac{\bar{\theta}}{2[1-(r/r_0)^2]}$$

$$\Rightarrow \frac{\theta}{\bar{\theta}} = \frac{1}{2\left[1-\left(\frac{r}{r_0}\right)^2\right]}$$

The fraction of stream in between r and r+dr

$dJ(r) = dJ(\theta) = \frac{u\,(2\pi r\,dr)}{Q}$ and has a residence between θ and $\theta + d\theta$. substituting

$$dJ(\theta) = \frac{4Q\,\pi r\,dr}{\pi r_0^2 Q}\left[1 - \left(\frac{r}{r_0}\right)^2\right] = \frac{4}{r_0^2}[1 -$$

Now,

$$d\theta = \frac{\bar{\theta}}{2}\left[\frac{-1}{\left[1-\left(\frac{r}{r_0}\right)^2\right]^2}\right]\left(-\frac{2r}{r_0^2}\right)dr$$

$$r\,dr = \frac{\bar{\theta}}{4\theta^2}\, r_0^2\, d\theta$$

$$\frac{dJ(\theta)}{d\theta} = \frac{1}{2}\frac{\bar{\theta}^2}{\theta^3} = J'(\theta) = E(t)$$

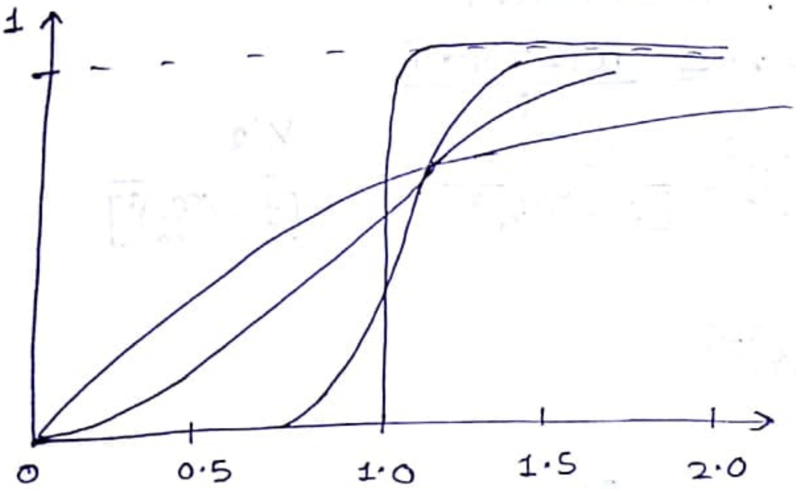
The minimum residence time is at not the centre where $u(r)$ is maximum

$$\theta_{min} = \frac{1}{2}\frac{V}{Q} = \frac{1}{2}\bar{\theta} \quad ; \quad \theta = \frac{V/Q}{2[1-(\frac{r}{r_0})^2]}$$

$$J(\theta) = \int_{\bar{\theta}/2}^{\theta} \frac{1}{2}\frac{\bar{\theta}^2}{\theta^3} d\theta = 1 - \frac{1}{4}\left(\frac{\theta}{\bar{\theta}}\right)^2 = F(t)$$

and

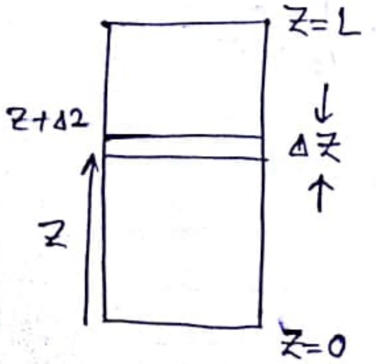
$$J'(\theta) = \frac{1}{2}\frac{\bar{\theta}^2}{\theta^3} = E(t)$$



One parameter models
- Dispersion
- CSTR in series model
- Recycle reactor model

Interpretation of Response data by the Dispersion model

- Dispersion takes place in a situation when there is an axial variation in velocity in a tubular reactor



- closed vessel is one in which, non ideality exists

$$\left[\left(-D_L\frac{\partial c}{\partial z} + uc\right)\pi r_0^2\right]_z \Delta\theta - \left[\left(-D_L\frac{\partial c}{\partial z} + uc\right)\pi \ldots\right]_{z+\Delta z}$$

$$= \left(c(\theta+\Delta\theta) - c(z)_\theta\right)\Delta z \, \pi r_0^2$$

$$\Rightarrow \boxed{+D_L \frac{\partial^2 c}{\partial z^2} - u\frac{\partial c}{\partial z} = \frac{\partial c}{\partial \theta}}$$

$$c = \begin{cases} 0 & \text{at } z>0 \text{ for } \theta=0 \\ c_0 & \text{at } z<0 \text{ for } \theta = 0 \end{cases}$$

at $z=0$, at feed no axial dispersion (closed vessel)

B.C $\quad z=0$, $\theta \geq 0$

$$-D_L\left(\frac{\partial c}{\partial z}\right)_{>0} + u(c)_{>0} = uc_0$$

$z>0$, just inside the reactor]

$z=L$, $\theta \geq 0$ $\quad \frac{dc}{dz} = 0$

Solution with this B.C is difficult

The diffn eqn is to be modified with

$$c^* = \frac{c}{c_0} \qquad \alpha = \frac{z-u\theta}{\sqrt{4D_L\theta}}$$

$$\text{B.C} = c^* = \begin{cases} 1 & \alpha = -\infty \\ 0 & \alpha = \infty \end{cases} \quad \text{as} \; \begin{vmatrix} c = c_0 \text{ at } z = -\infty \\ c = 0 \quad z = \infty \end{vmatrix}$$

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

[see B.S.L transport phenomena]

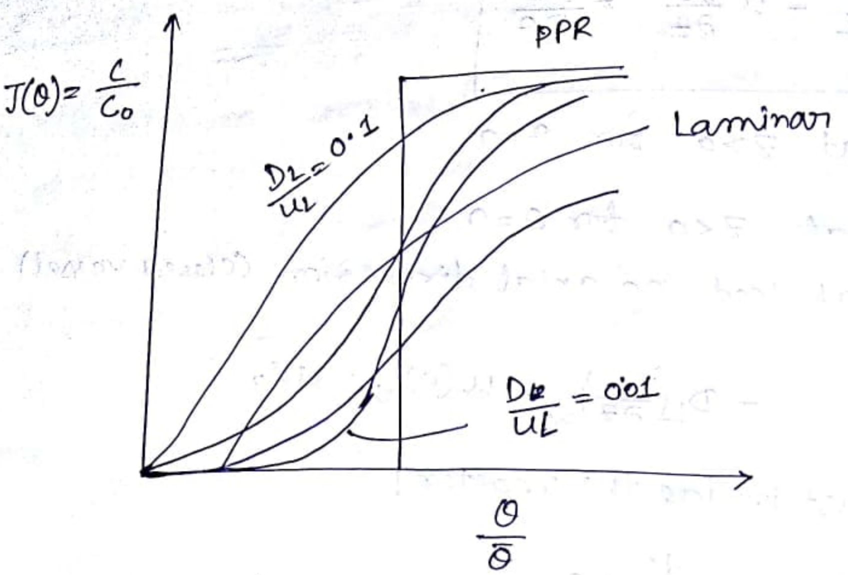
$$c^*_{z=L} = \left(\frac{c}{c_0}\right)_{\text{step}}$$

$$= \frac{1}{2}\left[1 - \text{erf}\left(\frac{1}{2}\sqrt{\frac{uL}{D_L}}\;\frac{1-\theta/\bar{\theta}}{\sqrt{\theta/\bar{\theta}}}\right)\right]$$

$\sqrt{\frac{1}{\text{Peclet no.}}}$

$$\bar{\theta} = \frac{L}{u}$$

$\therefore \frac{D_L}{uL}$ is the reciprocal of Peclet no. or vessel dispersion number



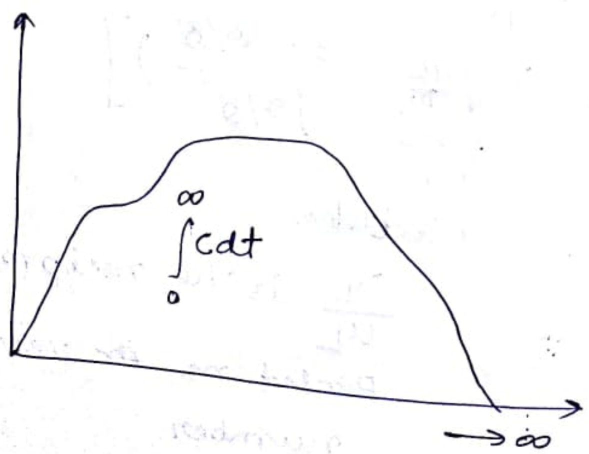
Identical reactor size
for 1^{st} order

$$\frac{C_A}{C_{Ap}} = 1 + (k\tau)^2 \frac{D}{uL} \quad \text{for same } V$$

n^{th} order reaction

$$\frac{C_A}{C_{Ap}} = 1 + n\left(\frac{D}{uL}\right)\left(kC_{A_0}^{n-1}\tau\right) \ln \frac{C_{A0}}{C_{AP}}$$

C vs θ only increases : step data
C vs θ first increases and then decreases : Pulse data



$\bar{C}_A = \int_{t=0}^{\infty}$ (

For 1^{st} ord

$C_{A,\text{elemen}}$

$\bar{C}_A = C$

$\bar{x} = \Sigma$ (
For a rea

$\bar{C}_A = C_A$

For inter

Stirred

C_0

Mole b

Assum

V_t

$$\bar{C}_A = \int_{t=0}^{\infty} C_{A,\text{element}}\, E\, dt$$

For 1st order assumption

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

$$\bar{C}_A = C_{A0} \int_0^{\infty} e^{-kt}\, E\, dt \rightarrow C_{A0} \sum e^{-kt} E \Delta t$$

$$\bar{x} = \sum (1 - e^{-kt}) E \Delta t \qquad \text{for CSTR } E = \frac{1}{\bar{\theta}} e^{-\theta/\bar{\theta}}$$

For a reversible 1st order rxn with no product in feed

$$\bar{C}_A = C_{A0} \int_0^{\infty} \left[1 - X_{Ae} + X_{Ae}\, e^{-kt/X_{Ae}}\right] E\, dt$$

For intermediate R in the succesive first order rxn

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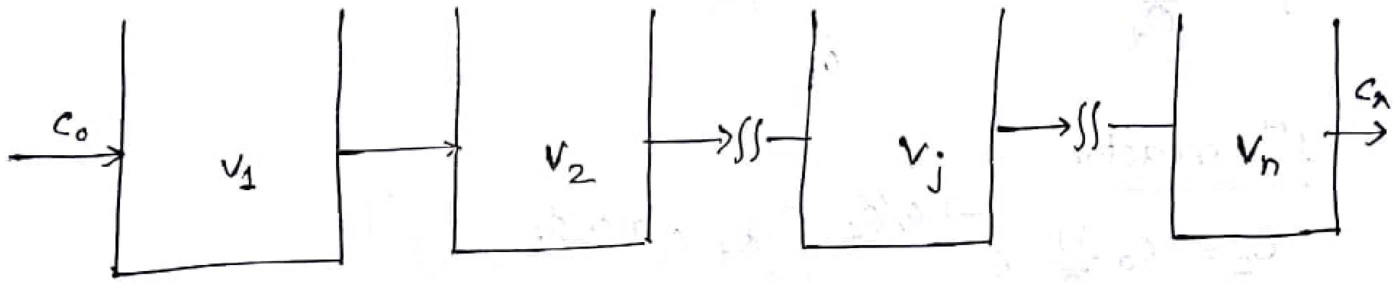
Stirred Tank in series model



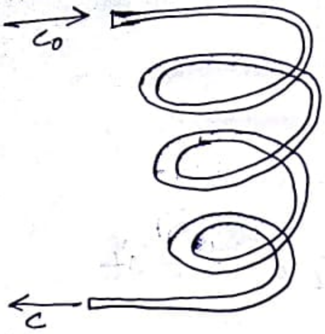
Mole balance over j^{th} reactor

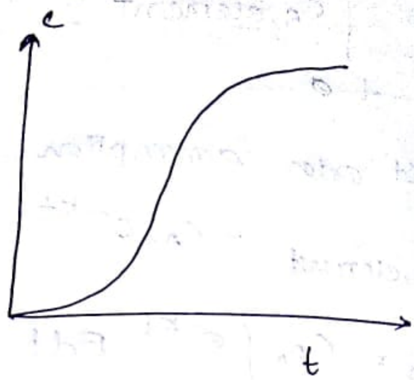
Assuming $V_1 = V_2 = \ldots\ V_j = V_N$

$$V_t = n V_j \qquad \bar{\theta}_t = \frac{V_j}{Q} \cdot n = \frac{V_t}{Q}$$

$$\frac{Q}{V_j} = \frac{n}{\bar{\theta}_t}$$

Actual reactor : Step input





$$c_{j-1} - c_j = \frac{V_j}{Q}\frac{dc_i}{d\theta}$$

$$\frac{dc_j}{d\theta} + \frac{n}{\bar{\theta}} c_j = \frac{n}{\bar{\theta}_t} c_{j-1}$$

$$\boxed{\frac{dy}{dx} + Py = Q}$$

at $\theta = 0, \quad c_j = 0$

$$c_j = \frac{n}{\bar{\theta}_t} e^{-n\theta/\bar{\theta}_t} \int_0^\theta c_{j-1} e^{n\theta/\bar{\theta}_t} d\theta$$

1st reactor

$$c_1 = c_0 \frac{n}{\bar{\theta}_t} e^{-n\theta/\bar{\theta}_t} \left[\frac{\bar{\theta}_t}{n} \left(e^{n\theta/\bar{\theta}_t} - 1\right) \right]$$

$$\boxed{\frac{c_1}{c_0} = 1 - e^{-n\theta/\bar{\theta}_t}}$$

2nd reactor

$$c_2 = \frac{n}{\theta_2} e^{-n\theta/\bar{\theta}_t} \int_0^\theta c_0 \left(1 - e^{-n\theta/\bar{\theta}_t}\right) e^{n\theta/\bar{\theta}_t} d\theta$$

$$\frac{c_n}{c_0} = J_n(\theta)$$

$$= 1 - e^{n\theta/\bar{\theta}_t} \left[1 + \frac{n\theta}{\bar{\theta}_t} + \frac{1}{2!}\left(\frac{n\theta}{\bar{\theta}_t}\right)^2 + \dots + \frac{1}{(n-1)!}\left(\frac{n\theta}{\bar{\theta}_t}\right)^{n-1} \right]$$

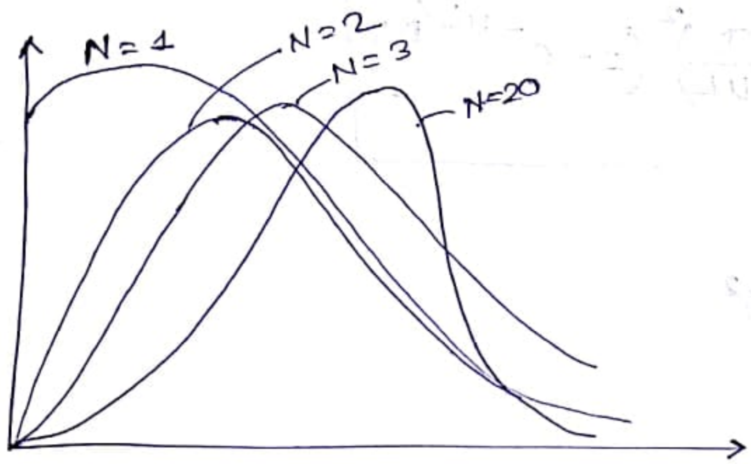
$$x_n = \left(1 - \frac{C_n}{C_0}\right) = 1 - \frac{1}{\left(1 + \frac{k\bar{\theta}_t}{n}\right)^n}$$

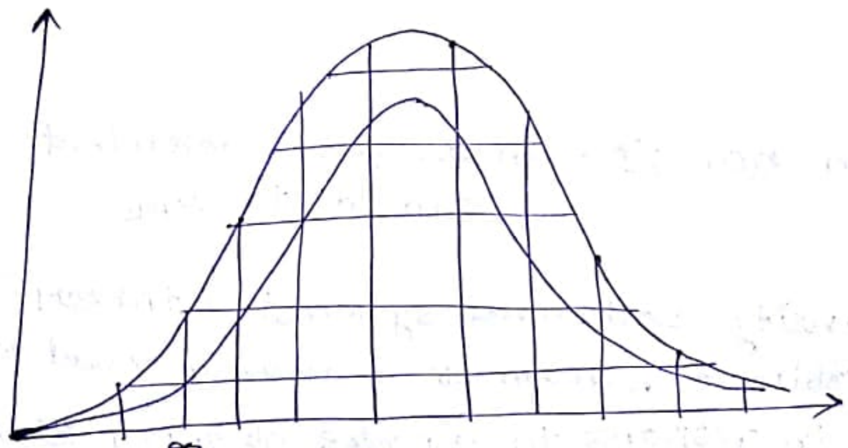
$N =$ Known

$$\frac{C_{A,N}}{C_{A,plug}} = 1 + \frac{(k\tau)^2}{N}$$

$$N = \frac{1}{\sigma_\theta^2}$$

Where σ_θ^2 = normalized variance





$$\sigma^2 = \frac{\int_0^\infty (t-\bar{t})^2 c\,dt}{\int_0^\infty c\,dt}$$

$$\sigma^2 \approx \frac{\int_0^\infty t^2 c\,dt}{\int_0^\infty c\,dt} - \bar{t}^2$$

$$\sigma^2 \cong \int_0^\infty t^2 E\,dt - \bar{t}^2$$

$$\bar{t} = \frac{\int_0^\infty t\,c\,dt}{\int_0^\infty c\,dt} = \int_0^\infty E\,dt$$

$$\bar{t} \cong \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i}$$

$$\cong \sum t_i E_i \Delta t_i$$

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

N = known

$$\frac{C_{A,N}}{C_{A,plug}} = 1 + \frac{(k\tau)^2}{N}$$

$$N = \frac{1}{\sigma_\theta'^2}$$

$\frac{D}{uL}$ = Dispersion no. ; D = dispersion coefficient similar to D_{AB}

Q|| For a constant density isothermal system, the tracer concentration in the effluent stream of a reactor vessel are obtained as follows in response to a pulse of tracer added to the feed

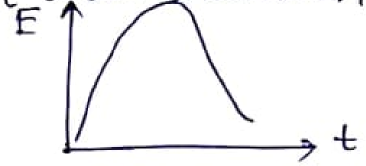
t, min	0	5	10	15	20	25	30	35
Tracer conc. g/c.c	0	3	5	5	4	2	1	0

a) Plot the exit age distribution curve (E vs. t)

b) Calculate the average residence time from tracer data

c) If the reactor as a closed vessel is well represented by dispersion model, calculate the vessel dispersion number D/uL

d) What conversion is expected if the conversion employing a plug flow reactor with the same residence time is 0.7 for first order reaction



$$Q = \int_0^\infty c\,dt = \sum c\,\Delta t = (3+5+5+4+2+1)\times 5 = 100\ \frac{g.min}{c.c}$$

$$\bar{t} = \sum t_i E_i \Delta t$$

t	5	10	15	20	25	30	35
E	0.03	0.05	0.05	0.04	0.02	0.01	0

$t = 15$ min

or $$\bar{t} = \frac{\int_0^\infty t\,c\,dt}{\int_0^\infty c\,dt}$$ if normalized data are not used

$$\sigma^2 = \frac{\int_0^\infty t^2 c\,dt}{\int_0^\infty c\,dt} - \bar{t}^2 = \frac{\sum t_i^2 c_i \Delta t_i}{\sum c_i \Delta t_i} - \bar{t}^2$$

in normalized form

$$\sigma^2 = \sum t_i^2 E_i \Delta t - \bar{t}^2 = \cancel{272.5}\ 47.5$$

$$\sigma_\theta^2 = \frac{\sigma^2}{\bar{t}^2} = \frac{47.5}{(15)^2} = 0.211$$

For closed vessel.

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

ignoring the second term

$$\sigma_\theta^2 = 0.211 = 2\frac{D}{uL}, \quad \frac{D}{uL} = 0.106$$

By trial and error

let, $\frac{D}{uL} = 0.106 \qquad \sigma_\theta^2 = 0.211 = 0.21099$

let $\frac{D}{uL} = 0.11$

$$\tau_p = \bar{t} = 15 \text{ min}$$

$$1 - 0.7 = e^{-(k \times 15)}$$

$$k = 0.08$$

$$N = \frac{1}{\sigma_\theta^2} = \frac{1}{\cancel{0.12}\ 0.211} = \cancel{8} \ 4.74$$

N should be 5

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Multiple Reactions

Example

Parallel: 1) $C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + Cl$

$C_6H_6 + 3Cl_2 \rightarrow C_6Cl_6$

2) $C_2H_6 \rightarrow C_2H_4 + H_2$

$C_2H_6 \rightarrow C_2H_2 + 2H_2$

3) $(CH_3)_2CHOH \rightarrow (CH_3)_2CO + H_2$

$(CH_3)_2CHOH \rightarrow CH_2CHCH_3 + H_2O$

1) Selectivity

2) Yield

3) Conversion

$A \rightarrow C$ $\quad k_1 C_A^{a_1}$ -- desired

$A \rightarrow D$ $\quad k_2 C_A^{a_2}$ -- undesired

50% A, 50% B

$A + B \rightarrow C$ $\quad -r_{A_1} = k_1 C_A C_B$

$A + B \rightarrow D$ $\quad -r_{A_2} = k_2 C_A C_B$

30 moles of A & 30 moles of B reacted to form 30 moles of C

10 moles of A & 10 moles of B react to form 10 moles of D

$$\text{selectivity of } C = \frac{\text{moles of C formed}}{\text{moles of D formed}} = \frac{30}{10} = 3$$

Yield of C

$$= \frac{\text{mole of C formed}}{\text{moles of A reacted}} = \frac{30}{50} \times 1000\,\% = 60\%$$

Conversion

$$= \frac{\text{Total A reacted}}{\text{Total A supplied}} = \frac{30+10}{50} \times 100\,\% = 80\%$$

* The yield of a reaction is defined as the ratio of moles of a desired product form to the maximum total amount of that species could be formed at 100% conversion level.

Parallel

<u>Qualitative Analysis</u>

$A \longrightarrow R$ $\quad k_1 C_A^{a_1}$ → Desired

$A \longrightarrow S$ $\quad k_2 C_A^{a_2}$

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

<u>Cases</u>: i) $(a_2 - a_1) = 0$: independent of conc.

ii) $(a_2 - a_1) \to +ve$: high conc. of A for more desired product

iii) $(a_2 - a_1) \to -ve$: Low conc. of A for more desired product

<u>again</u>

$A + B \longrightarrow R \qquad -r_{A_1} = k_1 C_A^{a_1} C_B^{b_1}$

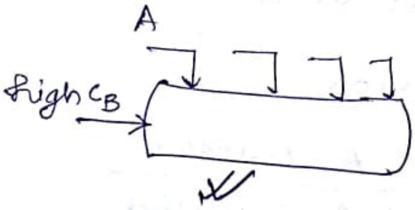
$A + B \longrightarrow S \qquad -r_{A_2} = k_2 C_A^{a_2} C_B^{b_2}$

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

	$(a_2 - a_1)$	$(b_2 - b_1)$
1	0	0
2	-ve	-ve
3	+ve	+ve
4	-ve	+ve
	+ve	-ve

e.g. $\frac{dC_R}{dt} = k_1 C_A C_B^{0.3} = r_R$

$\frac{dC_S}{dt} = k_2 C_A^{0.5} C_B^{1.8} = r_S$



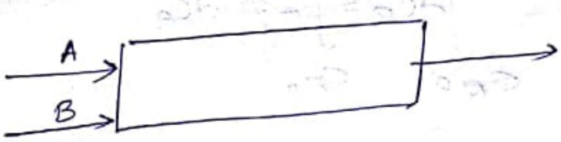
$$\frac{r_S}{r_R} = \frac{k_2}{k_1} C_A^{-0.5} C_B^{1.5}$$

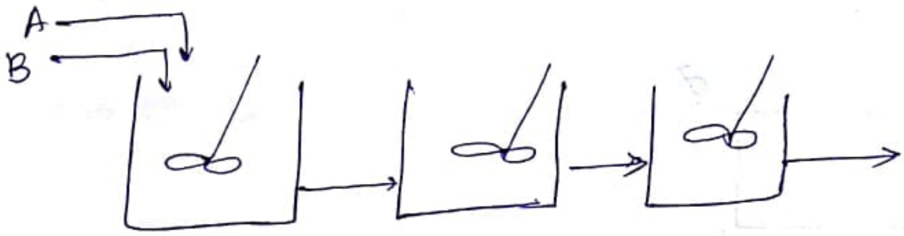
For more desired product, high conc. B and low conc. of A is required

$C_A \to$ low

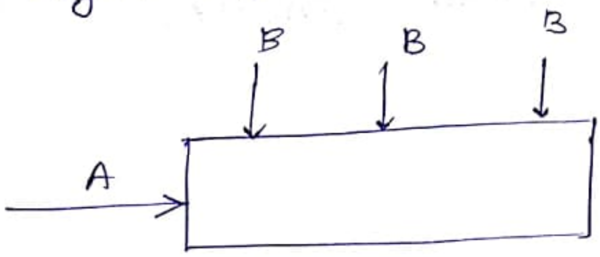
$C_B \to$ high

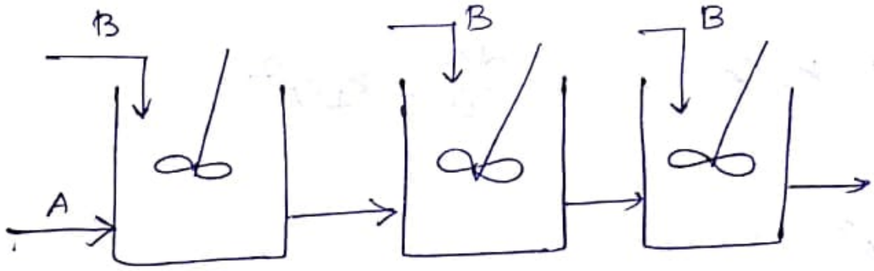
C_A, C_B both high

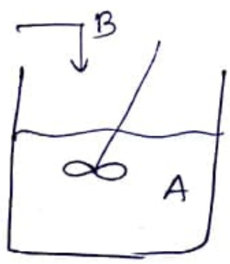




$C_A \rightarrow$ high, $C_B \rightarrow$ low





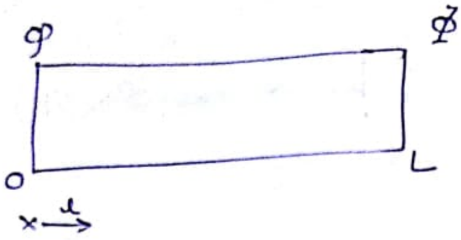


Semi-batch

Instantaneous fractional yield

$$\phi = \frac{dC_R/dt}{\text{total mole reacted } \left(-\frac{dC_A}{dt}\right)} = \frac{dC_R}{-dC_A}$$

$$\int_{0}^{C_{Rf}} dC_R = \int_{C_{A0}}^{C_{Af}} -\phi \, dC_A$$



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

$A \rightarrow R \quad k_1 C_A^2$

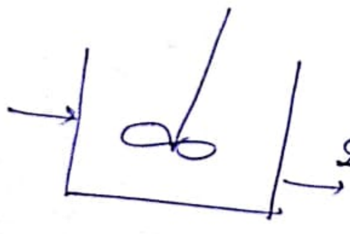
$A \rightarrow S \quad k_2 C_A$

$$-\frac{dC_A}{dt} = k_1 C_A^2 + k_2 C_A \qquad \frac{dC_R}{dt} = k_1 C_A^2$$

$$\phi = \frac{k_1 C_A^2}{k_1 C_A^2 + k_2 C_A^2}$$

in mixed reactor, $C_{Rf} = \phi (C_{A0} - C_{Af})$;

in PFR , $\phi = \frac{dC_R}{-dC_A} = -\int_{C_{A0}}^{C_{Af}} \phi \, dC_A$



$$\Phi = \bar{\phi}$$

Mixed flow reactor

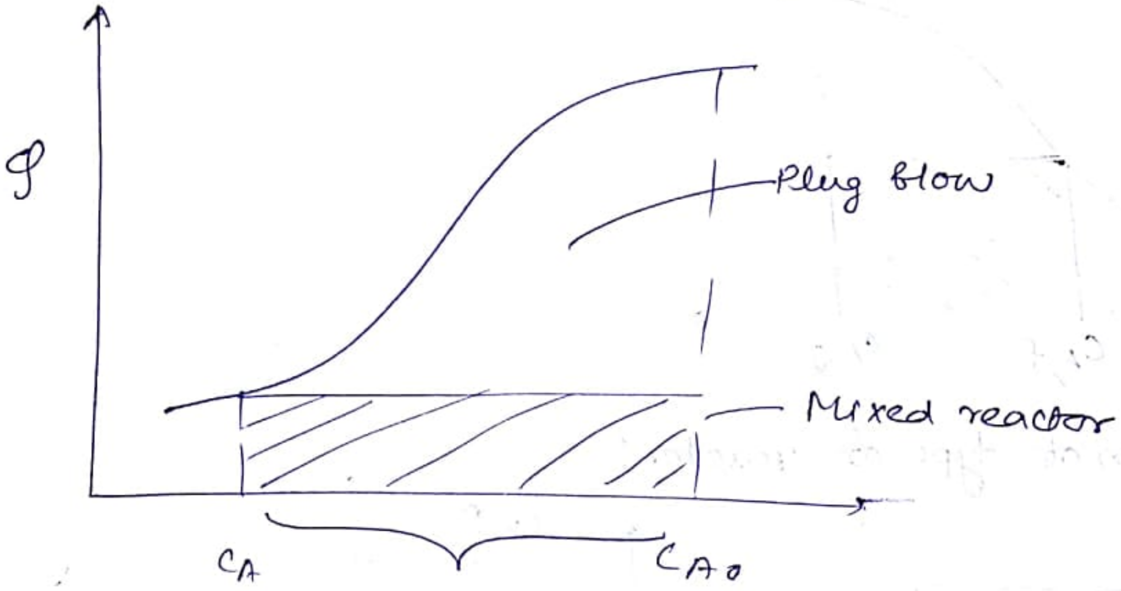
$$\bar{\phi}_m = \left(\frac{dC_R}{-dC_A}\right)_{\text{at } C_{Af}} = \phi \text{ evaluated at } C_{Af}$$

Plug flow reactor

$$\bar{\Phi}_p = \frac{-1}{C_{A0} - C_{Af}} \int_{C_{A0}}^{C_{Af}} \phi \, dC_A$$

C_{Rf} determination

$$\int_{C_{A0}}^{C_{Af}} \phi \, dC_A = \text{graphical integration and } \phi(C_{A0} - C_{Af}) = \text{rectangular area}$$

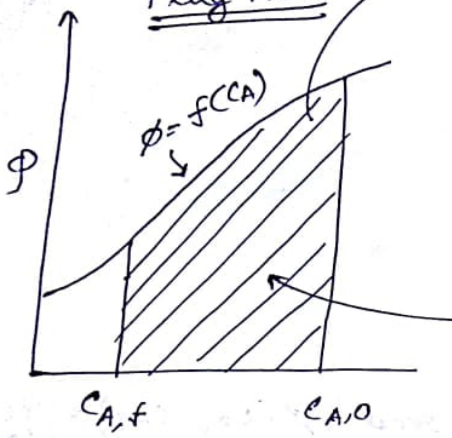


$$C_{Rf,m} = (-\Delta C_A)\,\bar{\phi}_m$$

$A \rightarrow R$ (desired)

$A \rightarrow S$

Plug Flow

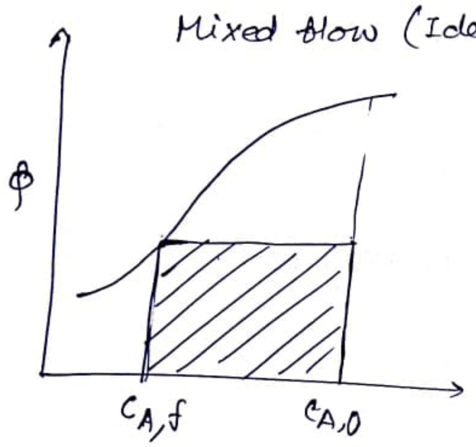


$$\int_{C_{A0}}^{C_{Af}} \phi \, dC_A$$

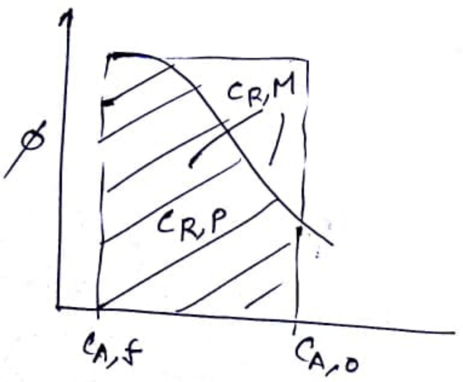
Instanteneous yield $\phi\left(\frac{R}{A}\right)$

$$\bar{\Phi}_P = \frac{-1}{C_{A0} - C_{Af}} \int_{C_{A0}}^{C_{Af}} \phi \, dC_A$$

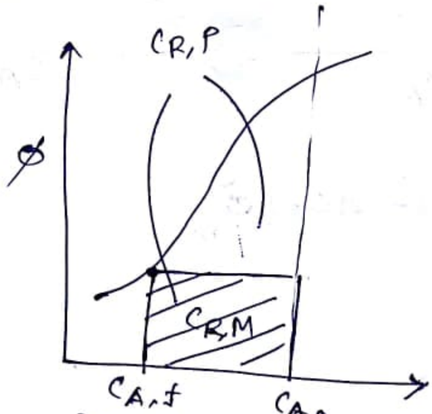
Mixed flow (Ideal CSTR)



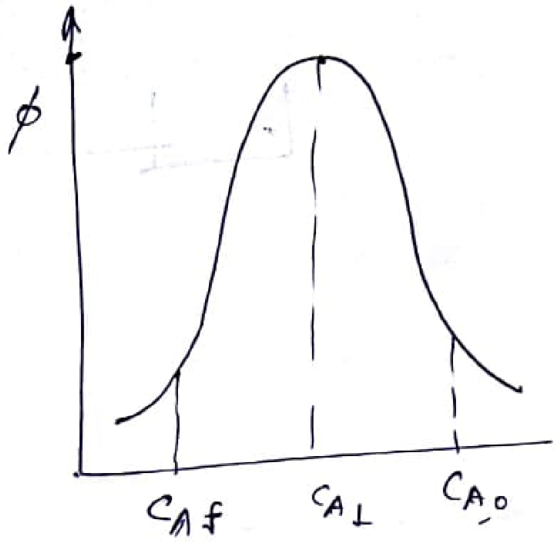
Selection of type of reactor:



Mixed flow reactor is best



PFR is best



combination of both PFR, mixed reactor

Q

$$A \to R,\quad A \to S \text{ (desired)},\quad A \to T$$

$r_R = 1$

$r_S = 2C_A$

$r_T = C_A^2$

$C_{A0} = 2$ mol/ltr.

$$\phi\left(\frac{S}{A}\right) = \frac{d[S]/dt}{\frac{d[R]}{dt} + \frac{d[S]}{dt} + \frac{d[T]}{dt}} = \frac{2C_A}{1 + 2C_A + C_A^2} = f(C_A)$$

Determine the maximum concentration of desired product (C_S) that can be obtained in

a) Mixed flow reactor

b) Plug flow reactor

Sol^n

$$\phi' = \frac{2C_A[\cancel{2}+2C_A] - [1+2C_A+C_A^2]2}{(1+2C_A+C_A^2)^2} = \frac{2C_A^2 - 2}{(1+C_A)^4}$$

$$\phi' = \frac{2(C_A^2-1)}{(1+C_A)^4}$$

$C_A = 1$ or $C_A = -1$ ✗ neglected

$$\phi_{max} = \frac{2}{(1+1)^2} = 0.5$$

$C_{s,f} = \Phi\left(\frac{S}{A}\right)(-\Delta C_A)$

For mixed reactor

$$C_{s,f} = \varphi\left(\frac{S}{A}\right)(-\Delta C_A)$$

$$= \frac{2C_A}{(1+C_A)^2}\cdot(C_{A_0} - C_A)$$

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

for $C_{s,f\,max}$,

$$\frac{dC_{s,f}}{dt} = \frac{(2-2C_A)(1+C_A)^2 - (2C_A - C_A^2)\,2\,(1+C_A)}{(1+C_A)^4} = 0$$

$$1 - C_A^2 - 2C_A + C_A^2 = 0$$

$$C_A = 0.5$$

$$C_{s,f,max} = \frac{2\times0.5\,(2-0.5)}{(1+0.5)^2} = \frac{1.5}{1.5^2} = \frac{1}{1.5}$$

$$C_{s,f,max} = 0.666\ \frac{mole}{L}$$

for PFR

$$\Phi = \frac{-1}{C_{A,0} - C_{A,f}}\int_{C_{A,0}}^{C_{A,f}} \varphi\, dC_A = \frac{C_{Bf}}{(C_{A_0} - C_{A,f})}$$

$$C_{Bf} = -\int_{C_{A,0}}^{C_{A,f}} \varphi\, dC_A$$

$$C_{Bf} = -\int_{C_{A,0}}^{C_{Af}} \cancel{\frac{2(C_A^2-1)}{}}\ \frac{2C_A}{(1+C_A)^2}\, dC_A$$

$C_{s,f} =$

$$C_{S,f} = -\int_{2}^{C_{A,f}} \frac{2(1+C_A) - 2}{(1+C_A)^2}\, dC_A$$

$$= \left[-\ln(1+C_A)^2\right]_2^{C_{A,f}} - \left[\frac{2}{1+C_A}\right]_2^{C_{A,f}}$$

$$= -2\left[\ln(1+C_{A,f}) - \ln(3)\right] - \left[\frac{2}{1+C_{A,f}} - \frac{2}{3}\right]$$

$$= -2\ln\left(\frac{1+C_{A,f}}{3}\right) - \frac{\cancel{6} - 2 - 2C_{A,f}}{3(1+C_{A,f})}$$

$$= -2\ln\left(\frac{1+C_{A,f}}{3}\right) - \frac{4 - 2C_{A,f}}{3(1+C_{A,f})}$$

$$\frac{dC_{S,f}}{dC_{A,f}} = 0$$

$$-\frac{2 \times 1/3}{\frac{1+C_{A,f}}{3}} + \frac{4}{3(1+C_{A,f})^2} + \frac{2}{(1+C_{A,f})} + \frac{2C_{A,f}}{(1+C_{A,f})^2} = 0$$

$$\Rightarrow -\frac{2}{(1+C_{A,f})} + \frac{2}{(1+C_{A,f})} + \frac{4 - 3C_{A,f}}{3(1+C_{A,f})^2} = 0$$

$$C_{A,f} = \frac{4}{3}$$

Q

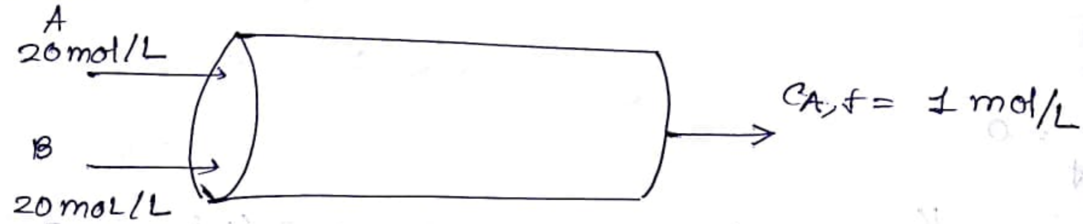
$$A + B \xrightarrow{k} R \text{, desired}$$

$$A + B \longrightarrow S$$

$$\frac{dC_R}{dt} = 1.0\, C_A C_B^{0.3} \quad mol/L.min$$

$$\frac{dC_S}{dt} = 1.0\, C_A^{0.5} C_B^{1.8} \quad "$$

Find the fraction of impurity in the product stream for 90% conversion of Pure A and B (each have a conc. of 20 mol/L) for a) plug flow reactor, b) mixed flow reactor, c) Plug-mixed combined C_B of dilute conc. of 1 mol/L.



soln

a)
$$\varphi = \frac{C_A C_B^{0.3}}{C_A C_B^{0.3} + C_A^{0.5} C_B^{1.8}}$$

$$\varphi = \frac{1}{1 + C_A^{-0.5} C_B^{1.5}}$$

$$\bar{\Phi}_p = \frac{-1}{C_{A_0} - C_{Af}} \int_{C_{A_0}}^{C_{Af}} \varphi \, dC_A$$

$$= \frac{-1}{10-1} \int_{10}^{C_{A,f}} \frac{dC_A}{1 + C_A} \qquad C_A = C_B$$

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

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

31/10/17

$$\Phi_p = \frac{R \text{ formed}}{A \text{ reacted}} = \frac{R \text{ formed}}{R \text{ formed} + S \text{ formed}}$$

$$1 - \Phi_p = 1 - 0.19 = 0.81 \equiv \text{fraction of } S$$

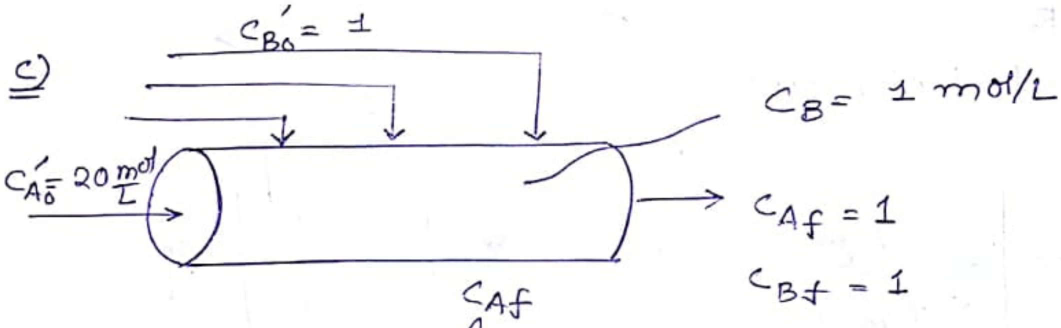
$$C_{Rf} = (C_{A_0} - C_{Af})\,\phi = 1.71 \text{ mol/L}$$

$$C_{Sf} = (C_{A_0} - C_{Af})(1-\phi) = 7.29 \text{ mol/L}$$

b) Mixed flow

$$\Phi_m = \phi_{at\ exit} = \frac{1}{1+C_{Af}} = \frac{1}{1+1} = 0.5$$

c)



$C_{A_0} = 19 \frac{mol}{L}$

$C_{B_0} = 1 \frac{mol}{L}$

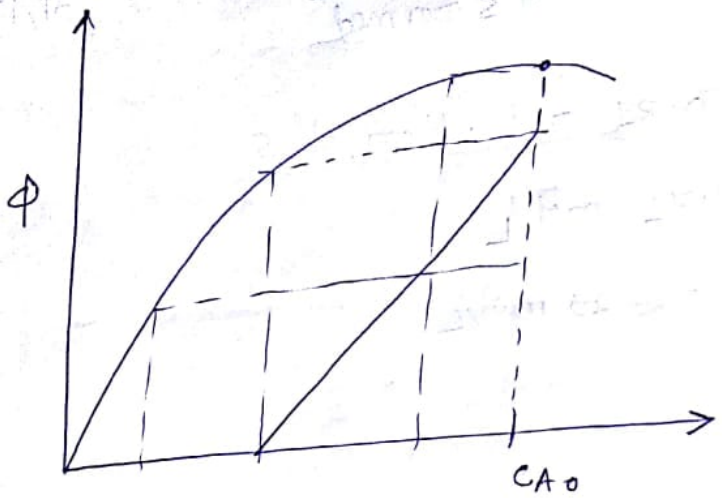
$$\Phi\left(\frac{R}{A}\right) = \frac{-1}{C_{A_0} - C_{Af}} \int_{C_{A_0}}^{C_{Af}} \phi \, dC_A$$

$$= \frac{-1}{19-1} \int_{19}^{1} \frac{dC_A}{1 + C_A^{-0.5}\, 1^{1.5}}$$

$$= \frac{1}{18}\left[(19-1) - 2(\sqrt{19} - 1) + 2 \ln \frac{1+\sqrt{19}}{2}\right]$$

$$= 0.741$$

F



$C_{R,f} = ?$

$$\frac{dC_{R,f}}{dC_A} = 0$$

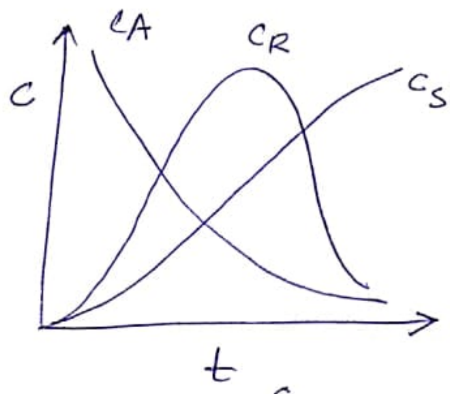
Series Reaction

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

$-r_A = \cancel{k} \, k_1 C_A$

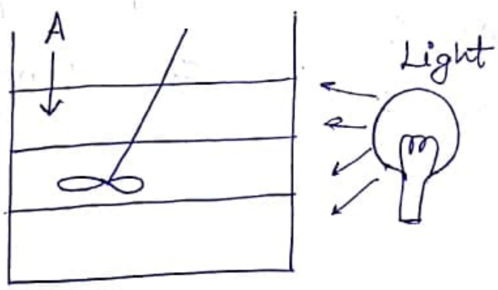
$r_R = k_1 C_A - k_2 C_R$

$r_S = k_2 C_R$

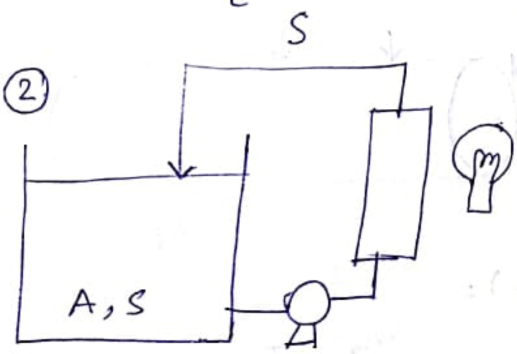


Some industrial techniques

(1)



(2)



- Mixed reactor is required to produce [S] maximum
- Plug flow " " " " " [R] maximum

Quantitative Analysis

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

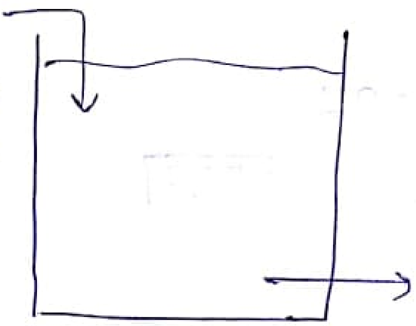
PFR

$$\frac{C_A}{C_{A0}} = e^{-k_1\tau} \qquad \frac{C_R}{C_{A0}} = \frac{k_1}{k_2-k_1}\left(e^{-k_1\tau} - e^{-k_2\tau}\right)$$

$$\frac{C_{R,max}}{C_{A0}} = \left(\frac{k_1}{k_2}\right)^{k_2/(k_2-k_1)} \qquad \tau_{p,opt} = \frac{\ln(k_2/k_1)}{k_2-k_1}$$

Mixed Flow

F_{A0}
$C_{R0} = 0$
$C_{S0} = 0$
C_{A0}
v_0



v
C_A
C_R
$C_S = C_{A0} - C_A - C_R$

A - balance

$$v C_{A0} = v C_A + k_1 C_A V$$

$$\frac{C_A}{C_{A0}} = \frac{1}{1+k_1\tau_m}$$

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

R - balance

$$v C_{R0} = v C_R + (-r_R)V$$

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

$$C_R\left(k_2 + \frac{1}{\tau_m}\right) = \frac{k_1 C_{A0}}{1+k_1\tau_m}$$

$$\frac{dC_R}{d\tau_m} = 0$$

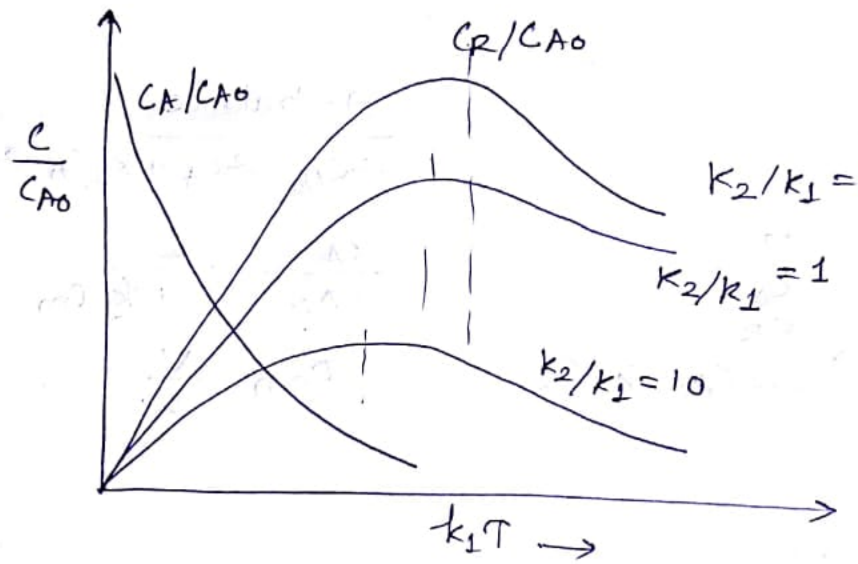
$$\boxed{\frac{C_R}{C_{A0}} = \frac{k_1\tau_m}{(1+k_1\tau_m)(1+k_2\tau_m)}}$$

$$\frac{dC_R}{d\tau_m} = \frac{C_{A0} k_1(1+k_1\tau_m)(1+k_2\tau_m) - C_{A0} k \tau_m \left[k_1(1+k_2\tau_m) + (1+k_1\tau_m)k_2\right]}{(1+k_1\tau_m)^2(1+k_2\tau_m)^2}$$

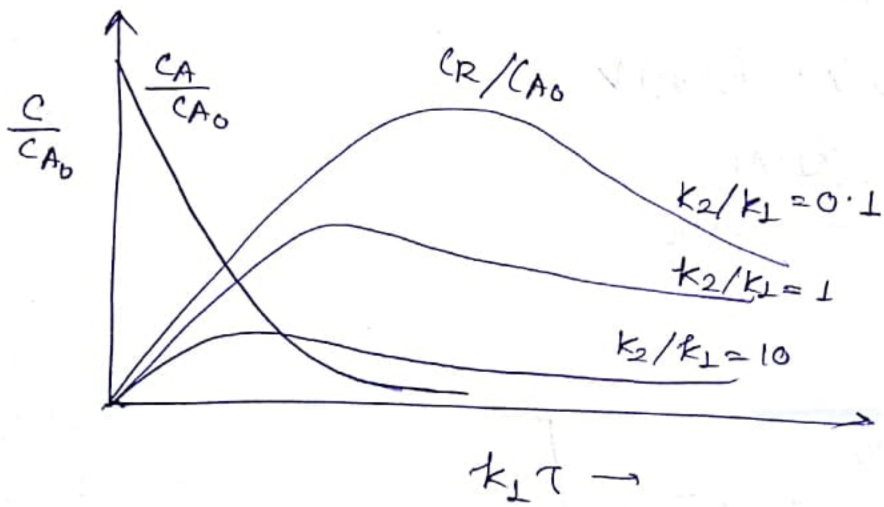
$$\tau_{m,opt} = \frac{1}{\sqrt{k_1 k_2}}$$

$$\frac{C_{R,max}}{C_{A0}} = \frac{1}{\left[\left(\frac{k_2}{k}\right)^{1/2} + 1\right]^2}$$

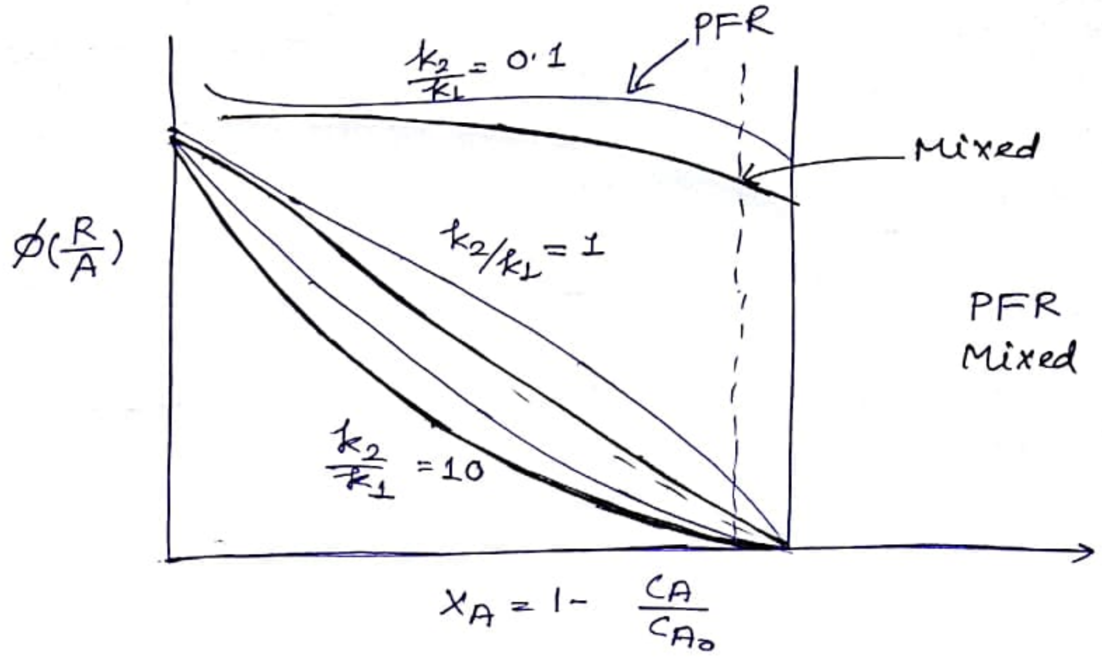
$$\boxed{\tau_{m,opt} = \frac{V_{opt.}}{v}}$$ → Design parameter



PFR



CSTR



- x_A is maintained at higher ~~conc~~. value for low $\frac{k_2}{k_1}$ ~~but~~ leading to larger ϕ
- x_A is maintained at lower value for higher $\frac{k_2}{k_1}$ leading to larger ϕ