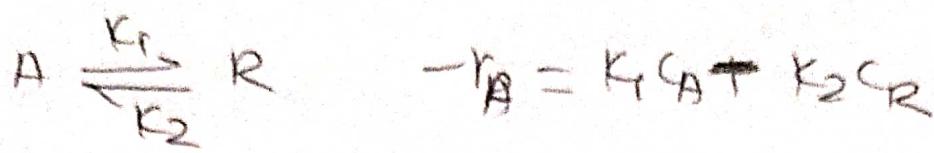


~~reversible~~

## # Reversible Rxns:

$$\text{At } m = \frac{C_{R_0}}{C_{A_0}}$$



$$-r_A = k_1 C_A - k_2 C_R = -\frac{dC_A}{dt} = C_{A_0} \frac{dx_A}{dt}$$

$$\text{At } C_R = C_{R_0} + C_{A_0} x_A, \quad C_A = C_{A_0} (1-x_A)$$

$$\therefore -\frac{dC_A}{dt} = k_1 C_{A_0} (1-x_A) - k_2 (C_{R_0} + C_{A_0} x_A)$$

$$-\frac{dC_A}{dt} = C_{A_0} \frac{dx_A}{dt} = k_1 C_{A_0} (1-x_A) - k_2 (C_{R_0} + C_{A_0} x_A) = -r_A$$

$$\frac{dx_A}{dt} = k_1 (1-x_A) - k_2 (m+x_A) \quad \text{--- (1)}$$

$$\frac{dx_A}{k_1 (1-x_A) - k_2 (m+x_A)} = dt$$

At eqbm,  $x_A = x_{eq}$  & net rate will be zero

$$\therefore -r_A = 0$$

$$k_1 (1-x_{eq}) = k_2 (m+x_{eq}) \Rightarrow \boxed{\frac{k_1}{k_2} = \frac{m+x_{eq}}{1-x_{eq}}}$$

$$k_1 - k_1 x_{eq} = k_2 m + k_2 x_{eq}$$

$$k_1 - k_2 m = (k_1 + k_2) x_{eq}$$

$$\therefore \boxed{x_{eq} = \frac{k_1 - k_2 m}{k_1 + k_2}}$$

where  $x_{eq}$  is  
eqbm conversion

$$\text{PF} \frac{K_1}{K_2} = \frac{m + \pi_e}{1 - \pi_e}$$

$$-r_A = -\frac{dC_A}{dt} = C_{AO} \frac{dx_A}{dt} = C_{AO} (K_1(1 - \pi_A) - K_2(m + \pi_A))$$

$$\frac{dx_A}{dt} = K_1(1 - \pi_A) - K_2 \frac{(1 - \pi_e)(m + \pi_A)}{(m + \pi_e)}$$

$$\frac{dx_A}{dt} = \frac{K_1(1 - \pi_A)(m + \pi_e) - K_2(1 - \pi_e)(m + \pi_A)}{(m + \pi_e)}$$

$$\frac{dx_A}{dt} = \frac{(K_1 m + K_2 \pi_e - K_1 \pi_A m - K_2 \pi_A \pi_e - K_1 m - K_2 \pi_A + K_1 \pi_e m + K_2 \pi_e \pi_A)}{(m + \pi_e)}$$

$$\frac{dx_A}{dt} = \frac{K_1(\pi_e - \pi_A m - \pi_A + \pi_e m)}{(m + \pi_e)}$$

~~$$\frac{dx_A}{dt} = K_1(\pi_e - \pi_A m - \pi_A + \pi_e m)$$~~

~~$$\frac{dx_A}{dt} = K_1(\pi_e - \pi_A m - \pi_A + \pi_e m + m - m)$$~~

$$\therefore \frac{dx_A}{dt} = K_1(\pi_e(1+m) - \pi_A(1+m))$$

$$\frac{dx_A}{dt} = \frac{k_f (2+m)(\gamma_e - \gamma_A)}{(m + \gamma_e)}$$

$$\int_0^{\gamma_A} \frac{d\gamma_A}{(\gamma_e - \gamma_A)} = \int_0^t \frac{k_f (2+m)}{(m + \gamma_e)} dt$$

$$(-\ln(\gamma_e - \gamma_A))_{\gamma_A} = \frac{k_f t (m+2)}{(m + \gamma_e)}$$

$$-\ln(\gamma_e - \gamma_A) + \ln \gamma_e = \square$$

$$\therefore \boxed{-\ln \left( \frac{\gamma_e - \gamma_A}{\gamma_e} \right) = k_f \frac{t (m+2)}{m + \gamma_e}}$$

Lect. 75

## variable volume batch reactor

$$r_p = \frac{1}{V} \frac{dN_p}{dt} = \frac{dc}{dt}$$

$$r_i = \frac{1}{V} \frac{d(C_i V)}{dt} = \frac{dc}{dt} + \frac{c}{V} \frac{dV}{dt}$$

$$\text{as } V = V_0(1 + \epsilon_A x_A)$$

For a rxn,



$$N_T = N_{T_0} + \delta N_{A_0} x_A, \quad \delta = \frac{(d+c) - (b+q)}{a}$$

$$\therefore \frac{N_T}{N_{T_0}} = 1 + \frac{N_{A_0} x_A}{N_{T_0}} \quad \textcircled{1}$$

$$\text{As } PV = N_T RT \text{ at time } t$$

$$\text{at initial time } P_0 V_0 = N_{T_0} R T_0$$

$$\therefore \frac{PV}{P_0 V_0} = \frac{N_T T}{N_{T_0} T_0} \Rightarrow$$

$$\Rightarrow V = V_0 \left( \frac{N_T}{N_{T_0}} \right) \left( \frac{T_0}{T} \right) \left( \frac{P_0}{P} \right) \quad \textcircled{2}$$

$$\text{But } Y_{A_0} = \frac{N_{A_0}}{N_{T_0}}$$

from eqn \textcircled{1} & \textcircled{2}

$$V = V_0 \left( \frac{P_0}{P} \right) \left( \frac{T_0}{T} \right) \left( 1 + \delta Y_{A_0} x_A \right)$$

$$\text{Now, } V = V_0 (1 + \varepsilon_A x_A) \left( \frac{P_0}{P} \right) \left( \frac{T}{T_0} \right)$$

At const. P & T

$$V = V_0 (1 + \varepsilon_A x_A)$$

$$A \rightarrow 3R$$

$$\varepsilon_A = \delta y_{A0}, \quad \delta = 2, \quad y_{A0} = \frac{1}{2} = \frac{1}{2}$$

$$\underline{\varepsilon_A = 2 \times \frac{1}{2} = 1}$$

$$\text{For } 50\% A, 50\% \text{ inert, } \delta = 2, \quad y_{A0} = \frac{0.5}{0.5+0.5} = 0.50$$

$$\therefore \varepsilon_A = 2 \times \frac{0.5}{1} = 1$$

$$\underline{\varepsilon_A = 1}$$

$$\varepsilon_A = \frac{V_{x_A=1} - V_{x_A=0}}{V_{x_A=0}}$$

$$\text{If } V_{x_A=1} = 3, \quad V_{x_A=0} = 1 \Rightarrow \varepsilon_A = \frac{3-1}{1} = 2$$

for 50% A & 50% inert.

$$V_{x_A=1} = 2.5, \quad V_{x_A=0} = 0.50 \Rightarrow \\ +0.5, \quad +0.50$$

$$\varepsilon_A = \frac{2.5 - 0.5}{1} = 2$$

② 40% of A & 60% of inert

Let basis 95 L mol

$$\Rightarrow \text{let } y_A = 0.40, y_I = 0.60$$

$$\therefore V_{x_A=0} = 2 \times 0.40 + 0.60 = 2$$

$$V_{x_A=2} = 0.40 \times 3 + 0.60 = 0.28$$

$$\therefore E_A = \frac{2.08 - 2}{2} = 0.08$$

$$\Delta N_A = N_{A_0} (1 - x_A)$$

$$\textcircled{2} \quad V = V_0 (1 + E_A x_A)$$

$$\Delta c_A = \frac{\Delta N_A}{V}$$

$$\therefore c_A = \frac{N_A}{V} = \frac{N_{A_0}(1 - x_A)}{V_0(1 + E_A x_A)} = \frac{c_{A_0}(1 - x_A)}{(1 + E_A x_A)}$$

$$\therefore \boxed{\frac{c_A}{c_{A_0}} = \left( \frac{1 - x_A}{1 + E_A x_A} \right)}$$

$$-r_A = -\frac{1}{V} \frac{dN_A}{dt} = \frac{c_{A_0}}{(1 + E_A x_A)} \frac{dx_A}{dt}$$

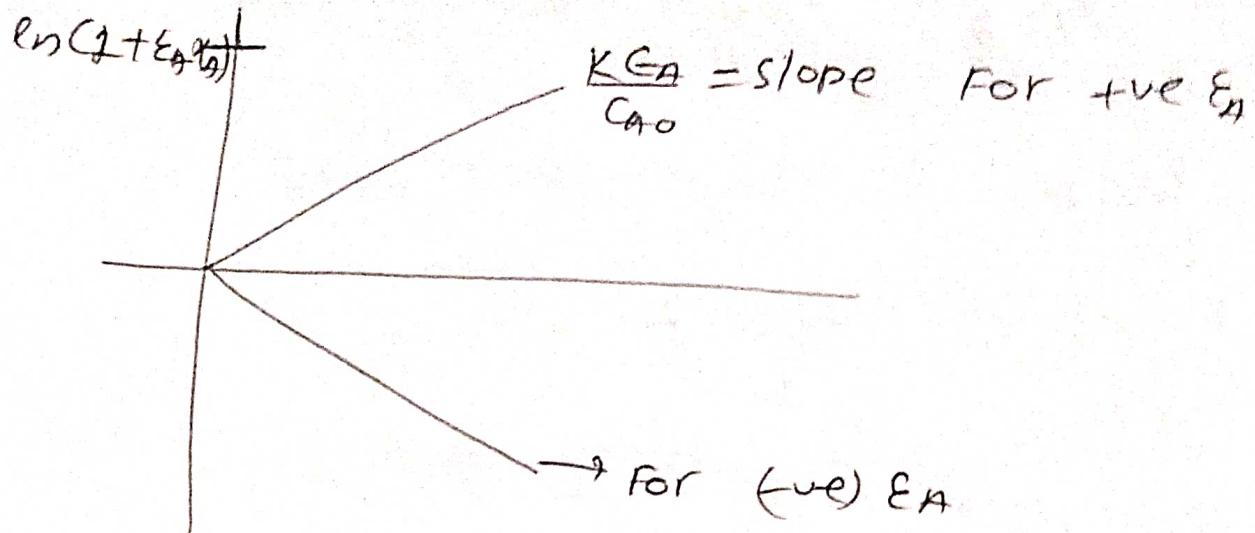
zero order Rxn -

$$-r_A = \frac{c_{A_0}}{(1 + E_A x_A)} \frac{dx_A}{dt} = k$$

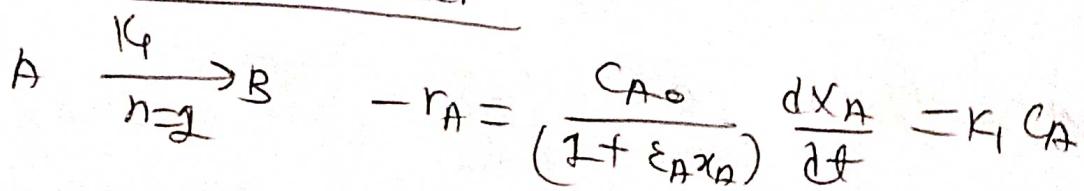
$$\therefore c_{A_0} \int_0^{x_A} \frac{dx_A}{(1 + E_A x_A)} = \int_0^t k dt$$

$$\frac{C_{A0}}{E_A} \ln(1 + E_A x_A) = k_f t$$

$$\therefore \boxed{\ln(1 + E_A x_A) = \left(\frac{k_f}{C_{A0}}\right) t}$$



For first order



$$\text{for VVRs, } C_A = \frac{C_{A0}(1 - x_A)}{(1 + E_A x_A)}$$

$$\therefore \frac{C_{A0} dx_A}{(1 + E_A x_A) dt} = k_f \times \frac{C_{A0}(1 - x_A)}{(1 + E_A x_A)}$$

$$\Rightarrow \int_0^{x_A} \frac{dx_A}{(1 - x_A)} = k_f dt$$

$$\ln(1 - x_A) = -k_f t$$

$$\text{OR } \boxed{x_A = 1 - e^{-k_f t}}$$

some of CVRD

Q. 1.

Show that the following position of  $N_{205}$  at  
67°C is a 1st order  $R/T^n$ , and the value of  
rate const.

Time(min) 0 1 2 3 4

$C_{N_{205}}$	0.76	0.113	0.08	0.056	0.040
---------------	------	-------	------	-------	-------

$$\rightarrow -\ln N_{205} = K (C_{N_{205}})^n = \frac{dC_n}{dt}$$

For 1st order  $C_{N_0} = 0.76, C_{N_1} = 0.113$

$$\frac{dC_n}{dt} = 0.047, dt = 1$$

Let it is a first order  $R/T^n$

$$\text{then } -\ln \left( \frac{C_n}{C_0} \right) = k_1 t$$

$$\Rightarrow -\ln \left( \frac{0.113}{0.76} \right) = k_1 \times 1 \Rightarrow k_1 = 0.3477$$

Again

$$\Rightarrow -\ln \left( \frac{0.08}{0.76} \right) = k_2 \times 2 \Rightarrow k_2 = \frac{0.6932}{2} \Rightarrow k_2 = 0.3465$$

$$-\ln \left( \frac{0.056}{0.76} \right) = k_3 \times 3 \Rightarrow k_3 = 0.3499$$

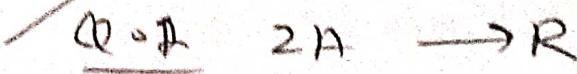
$$\text{or } -\ln \left( \frac{0.056}{0.08} \right) = k_3 \times 1 \Rightarrow k_3 = 0.3566$$

As all the  $k_1, k_2, k_3$  are very close to each other.

So, If it is a first order  $R/T^n$ ,

$$K_{avg} = 0.3476$$

Q. 16



80% A & 20% inert.  
 $0.8$                $0.2$

First order

Rxn

$$\therefore \varepsilon_A = \frac{V_{x_A=1} - V_{x_A=0}}{V_{x_A=0}} = \frac{0.6 - \cancel{0.2}}{\cancel{0.2}} = 0.6 - 0.2 = 0.4$$

$$\varepsilon_A = -0.4$$

$$V = V_0 (1 + \varepsilon_A x_A)$$

$$V = 0.8 V_0$$

$$0.8 = 1 - 0.4 x_A \Rightarrow 0.4 x_A = 0.2$$

$$\boxed{x_A = 0.5}$$

$$\therefore x_A = \frac{1}{2} = 0.5$$

for first order

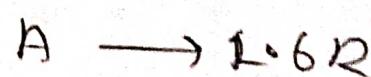
$$\ln(1 - x_A) = kt \Rightarrow -\ln(0.5) = kx_A t$$

$$kx_A t = 0.693$$

$$\text{As } t = 3 \text{ min}$$

$$\therefore k = \frac{0.693}{3} = 0.231 \text{ min}^{-1}$$

Q. 17 Find the 1st order rate const. for the  
dis. of A in the gas phase Rxn



If the volume of Rxn mix. starting with  
bure A increase by 50% 4 min. Total pressure  
within the system stay const. 20 atm  
if temp. is  $25^\circ C$ .

$$\epsilon_A = \frac{U_{A,n=2} - U_{A,n=0}}{U_{A,n=0}} = \frac{1.06 - 1}{1} = 0.06$$

$$V = 1.5 U_0 = U_0 (1 + 0.06 x_A)$$

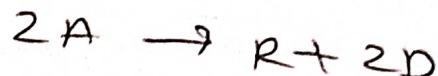
$$\frac{0.5}{0.6} = x_A \Rightarrow x_A = 0.833$$

$$P_A - \ln(1 - x_A) = k \times t = 1.789$$

$$K = 0.447 \text{ min}^{-1}$$

$$K = 7.45 \times 10^{-3} \text{ sec}^{-1}$$

③ A gas phase rxn



is second order  $Rx^n$  wrt A. If pure A is introduced at 1 atm into a const. volume batch reactor, the pressure rises by 40% in 3 min. In case of a const. - pr. batch reactor.

Find ① time required to achieve the same conversion

② The fractional increase in volume at that time

Note - at variable pressure  $\Rightarrow$  const. volume



$$P_0 = P_B = 1 \text{ atm}$$

At  $t = 3 \text{ min}$ ,  $P = 1.4 P_0 = 1.4 \text{ atm}$

$$P_A = P_{B_0} - \frac{a}{b n} (P - P_0)$$

$$P_A = 1 - \frac{2}{2} (1.4 - 1) = 0.2 \text{ atm}$$

$$\boxed{P_A = 0.2 \text{ atm}}$$

$$P_A = P_{A_0} (1 - x_A)$$

$$1 - x_A = \frac{0.2}{1} = 0.2$$

$$\boxed{x_A = 0.8}$$

$$P = P_0 (1 + \varepsilon_A x_A) = 1.4 P_0 \quad \left| \begin{array}{l} \varepsilon_A = \frac{3-2}{2} \\ 1 + \varepsilon_A x_A = 1.4 \end{array} \right.$$

$$1 + 0.5 x_A = 1.4 \quad \Rightarrow 0.5$$

$$x_A = \frac{0.4}{0.5} = 0.8$$

$$\boxed{x_A = 0.2}$$

Q2 For variable system —

$$\frac{(1 + \varepsilon_A) x_A}{1 - x_A} + \varepsilon_A \ln(1 - x_A) = K C_{A_0} x_A$$

$$\frac{1.5 \times 0.8}{0.2} + 0.5 \times \ln(0.2) = KC_{A_0}x + t$$

$$6 + 0.8047 = KC_{A_0}x + t$$

$$\textcircled{*} \quad 5.1953 = KC_{A_0}x + t = K \frac{x P_{A_0}}{RT} x + t \quad \textcircled{1}$$

(vrs)

$$\text{PF} \quad \frac{x_P}{1-x_A} = KC_{A_0}x + t \Rightarrow \frac{0.8}{0.2} = KC_{A_0}x + 3$$

$$KC_{A_0} = \frac{4}{3}$$

$$\therefore 5.1953 = \frac{4}{3}x + t$$

$$t = \frac{5.1953 \times 3}{4} = 3.896$$

$$\boxed{t = 3.896 \text{ min}}$$

$$\textcircled{2} \quad V = V_0(1 + \epsilon_A x_A) = V_0(1 + 0.05 \times 0.8) = 1.4V_0$$

$$\boxed{V = 1.4V_0} \Rightarrow 40\% \text{ increase in volume}$$

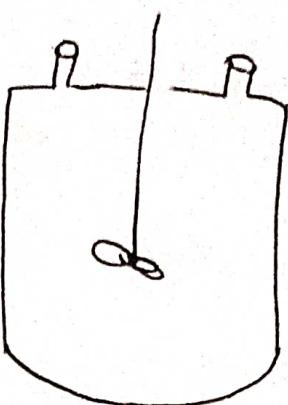
lect-27

## Design of Reactor

### ① Batch reactor:

$$\text{At } t=0, C_A = C_{A0}$$

$$X_A = 0$$



$$\text{At } t=t, C_A = C_A(t)$$

$$X_A = X_A(t)$$

$$\text{Input}^0 = \text{output}^0 + \text{disappearance} + \text{accumulation}$$

Rate of loss  
of A during  
rxn

$$= - \left( \begin{array}{l} \text{Rate of accumulation} \\ \text{or A within Reaction} \end{array} \right)$$

$$(-r_A \cdot v) = -\frac{dN_A}{dt}$$

$$r_A = \frac{\text{mol/time}}{\text{volume}}$$

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

$$\Rightarrow dN_A = -N_{A0} dX_A$$

$$(r_A \cdot v) = N_{A0} \frac{dX_A}{dt}$$

$$\int_0^t dt = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A \cdot v)}$$

$$\therefore t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A \cdot v)}$$

For both CURS  
& VURS.

General performance eqn of  
ideal batch reactor.

For CSTR,  $v = v_0 \rightarrow \frac{N_{A0}}{v_0} = c_{A0}$

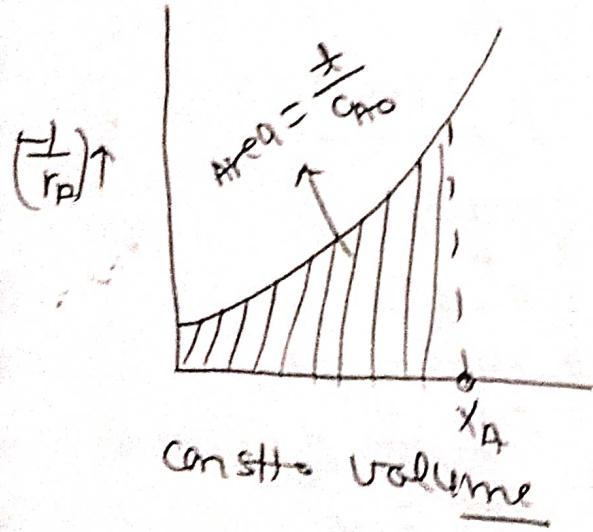
$$\therefore t = \frac{c_{A0}}{r_A} \int_0^{x_A} \frac{dx_A}{(1+r_A x_A)} \quad \text{--- (2)}$$

For WPS,  $v = v_0(1+r_A x_A)$  again  $\frac{N_{A0}}{v_0} = c_{A0}$

$$t = \frac{c_{A0}}{r_A} \int_0^{x_A} \frac{dx_A}{(1+r_A x_A)(-r_A)} \quad \text{--- (2)}$$

Here  $t$  = reaction time,

$$t_{\text{batch}} = t_{\text{exn}} + t_{\text{loading}} + t_{\text{unloading}}$$

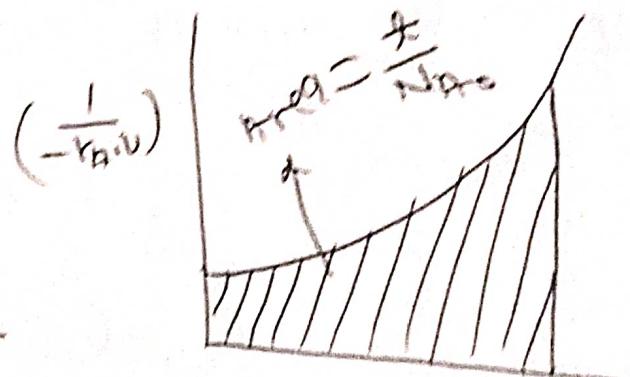


const. volume

$$c_A = c_{A0}(1 - r_A x_A)$$

$$dc_A = -c_{A0} dr_A$$

→ composition is uniform at a given time throughout the reactor.



In integration is there  
in eqn, so area under  
the curve will be  
considered.

## # Flow reactor

$$S = \frac{1}{\tau}$$

① Space time — time required to process reactor volume at ~~specified~~ of feed.

$$\tau = \frac{V}{V_0}$$

② space velocity —

$$S = \frac{V_0}{V}$$

$V$  = reactor volume

$V_0$  = volumetric flow rate

- Number OR volume reactor required to process ~~for~~ unit time

## Lecto 18

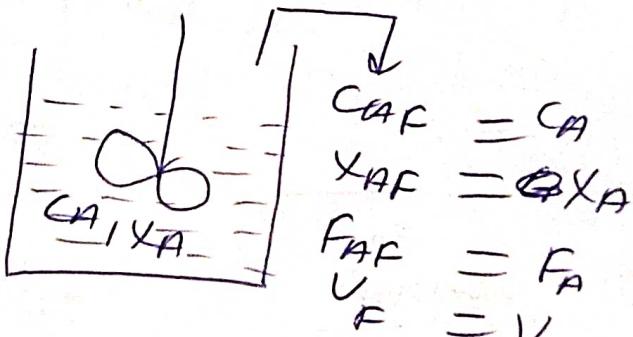
### Steady state mixed CSTR flow Reactor

$$C_{A0}, F_{A0}$$

$$x_{A0} = 0$$

$$V_0$$

$$\leftarrow V_0 = \text{volumetric flow rate}$$



In case of ideal mixed flow ~~reactor~~ reactor

$C_{A0} = C_{AF}$  (exit conc. will be uniform to mixer concentration)

material balance —

Input = output + disappearance + accumulation

I ded

characteristic of mixed flow reactor or CSTR:

→ The composition (concentration) is uniform at a given time throughout the reactor. (In the exit & in the reactor or reaction mixture).

→ In but = output + disappearance + Accumulation  
 steady state

$$F_{A0} = F_A + (-r_A V) + 0$$

$$\text{As } F_A = F_{A0} (1 - \chi_A)$$

$$\therefore F_{A0} = F_{A0} (1 - \chi_A) + (-r_A V)$$

$$F_{A0} (1 - 1 + \chi_A) = - r_A \cdot V$$

$$F_{A0} \chi_A = - r_A \cdot V$$

$F_{A0}$  = initial

molar flow rate

$$\boxed{\frac{V}{F_{A0}} = \frac{\chi_A}{(-r_A)}} \quad \textcircled{1}$$

$$\text{i.e. } F_{A0} = C_{A0} V_0$$

$$\frac{\text{mole}}{\text{time}} \rightarrow \frac{\text{mole}}{\text{mole} \times \frac{\text{mole}}{\text{time}}}$$

$$\frac{V}{C_{A0} V_0} = \frac{x_A}{(-r_A)} \rightarrow \text{reactor volume}$$

$\Delta L \frac{V}{V_0} = \tau$  → volumetric flow rate

∴ 
$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{x_A}{(-r_A)}$$

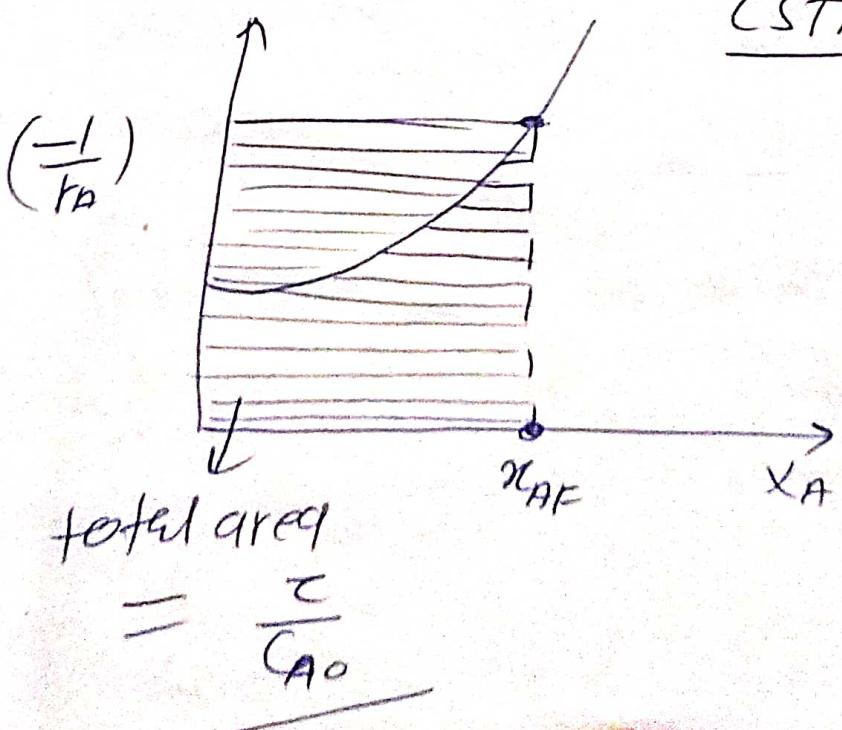
$$\tau = \frac{V}{V_0} = \frac{C_{A0} x_A}{(-r_A)}$$

As  $C_A = C_{A0} (1 - x_A) = C_{A0} - C_{A0} x_A$

∴  $C_{A0} x_A = C_{A0} - C_A$

∴ 
$$\tau = \frac{V}{V_0} = \frac{C_{A0} x_A}{(-r_A)} = \frac{(C_{A0} - C_A)}{(-r_A)}$$

↓  
performance eqn for  
CSTR.



As integration is  
not there in  
eqn so we have  
to consider  
total area (not  
only area  
under the curve)

Dontkoer

Dam Kohler

## # Mach number ( $D_g$ )

- It gives the idea about the conversion i.e. whether we are getting low conversion or high conversion.

$$D_g < 0.2$$

$$x_A < 20\%$$

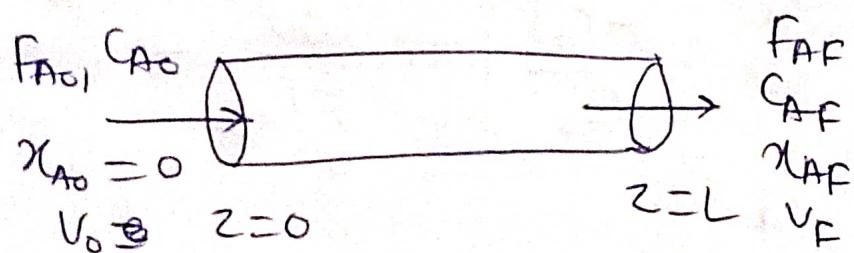
$$D_g > 10$$

$$x_A > 90\%$$

(PFR)

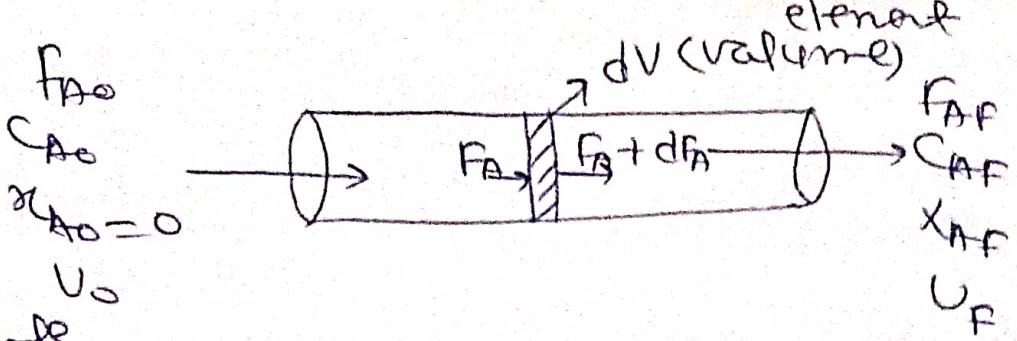
### ③ Steady state Plug Flow reactor:

- Back mixing is not allowed in PFR
- Composition varies along the length (path) of the reactor.



- ~~Each~~ each & every molecule of fluid particles having same residence time in case of PFR.

∴ Radial mixing =  $\infty$ , Axial mixing = 0  
 $\Rightarrow$  flat velocity profile.



mole Balance -

$$\text{Input} = \text{Output} + \text{disappearance}$$

$$F_A = (F_A + dF_A) + (-r_A) \times dV$$

$$\boxed{\frac{dF_A}{dV} = (-r_A)}$$

Rate of dis. of species A in  $dV$  volume.

→ performance eqn for PFR

$$\text{PFR} \quad F_A = F_{AO}(1 - x_A)$$

$$dF_A = -F_{AO}dx_A$$

$$\therefore \frac{F_{AO}dx_A}{dV} = (-r_A)$$

OR

$$\boxed{\frac{dx_A}{dV} = \frac{(-r_A)}{F_{AO}}}$$

$$\Rightarrow \int_0^V \frac{dV}{F_{AO}} = \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$\boxed{\frac{V}{F_{AO}} = \int_0^{x_A} \frac{dx_A}{(-r_A)}}$$

→ performance eqn for PFR

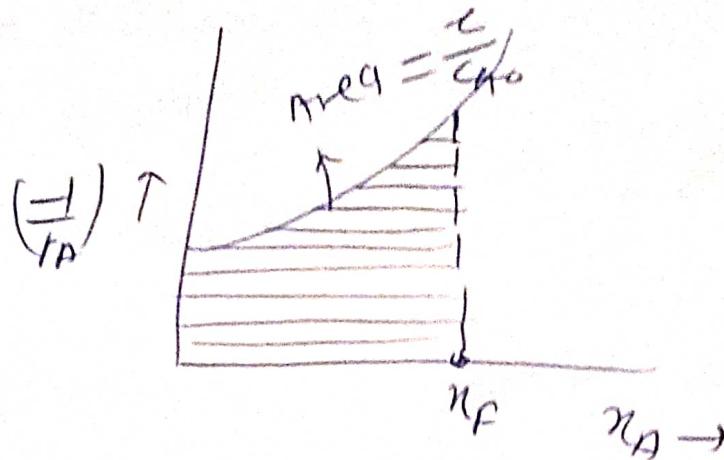
NOW,

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{x_A} \frac{dx_A}{(-r_A)}$$

Area under the

$$\text{curve} = \frac{\tau}{C_{A0}}$$

$$\text{or } \frac{V}{F_{A0}}$$



→ case ① for

$$e_n = 0,$$

constant rel. of first order

$$-r_A = k C_A = k C_{A0} (1 - x_A)$$

$$\therefore \frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{x_{A0}} \frac{dx_A}{k C_{A0} (1 - x_A)}$$

$$\therefore K\tau = -\ln(1 - x_A)$$

$$K\tau = -\ln(1 - x_A)$$

$$\therefore \tau = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)}$$

$\tau$  = space time  
PFR

$$t = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)}$$

$t$  = batch reaction  
time  
in BATCH REACTOR

## # Dam Kohler number ( $D_q$ )

(lect 9)

$D_q = \frac{\text{Rate of rxn at entrance}}{\text{convective or entering flow rate} \times \text{rate of A.}}$

$$D_q = \frac{(-r_A) \cdot V}{F_{A0}}$$

Here  $(-r_A) \rightarrow$  at entry condition

→ For First order

$$D_q = \frac{K C_{A0} \cdot V}{F_{A0}} \quad \text{As } F_{A0} = C_{A0} V_0$$

$$\therefore D_q = \frac{K C_{A0} V}{F_{A0}} = K \tau$$

$$\tau = \frac{V}{V_0} = \frac{C_{A0} V}{F_{A0}}$$

→ For second order rxn

$$D_q = \frac{K C_{A0}^2 V}{F_{A0}} = K C_{A0} \tau$$

In General

$$D_q = K C_{A0}^{n-1} \tau$$

$n = \text{order of the rxn.}$

for CSTR:

$$\frac{V}{F_{A_0}} = \tau = \frac{x_A}{C_{A_0}} \quad \text{OR} \quad \tau = \frac{C_{A_0} x_A}{(-r_A)}$$

For First order Rxn -

$$-r_A = k C_{A_0} = k C_{A_0} (1-x_A)$$

$$\tau = \frac{C_{A_0} x_A}{k C_{A_0} (1-x_A)} = \frac{x_A}{k (1-x_A)}$$

∴  $\boxed{k\tau = \frac{x_A}{1-x_A}}$  OR  $\boxed{x_A = \frac{k\tau}{1+k\tau}}$

Here  $k\tau = \frac{x_A}{1-x_A} = D_a$

$$\boxed{x_A = \frac{D_a}{1+D_a}}$$

Ques In an isothermal batch reactor, 70% of a liquid reactant is converted in 23 min. what space time & space velocity are needed to effect this conversion in a plug flow reactor and in a mixed flow reactor.

M.S for batch reactor

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

Let it is a first order rxn

$$-r_A = K C_A = K C_{A0} (1 - x_A)$$

$$t = C_{A0} \int_0^{x_A} \frac{dx_A}{\frac{K C_{A0} (1 - x_A)}{K C_{A0} (1 - x_A)}} = \frac{1}{K} (-\ln (1 - x_A))$$

$$t = \frac{1}{K} \times (-\ln (1 - x_A))$$

~~if~~  $x_A = 0.70 \quad 1 - x_A = 0.30$

$$t = \frac{2.204}{K}$$

$$K = \frac{2.204}{13} \text{ min}^{-1} = 0.0926 \text{ min}^{-1}$$

NOW, For PFR -

$$\tau = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)} = K C_A$$

Again for first order  $-r_A = K C_{A0} (1 - x_A)$

$$K \tau = \int_0^{x_A} \frac{dx_A}{(1 - x_A)} = -\ln (1 - x_A)$$

$$\Rightarrow \tau = 13 \text{ min}$$

$$\tau (\text{Space time}) = 13 \text{ min} \quad \text{For PFR}$$

$$\tau = \frac{1}{S} \therefore \text{Space velocity } S = \frac{1}{13} = 0.076 \text{ min}^{-1}$$

(2) Mixed Flow Reactor OR CSTR:

$$\text{Pf } \tau = \frac{C_{A0} x_A}{-r_A} = \frac{C_{A0} x_A}{K \cancel{T} x_0 (1-x_A)}$$

$$\tau = \frac{0.7}{(1-0.7)K} = \frac{0.7}{0.3 \times 0.0926} = \frac{0.7}{0.3 \times 0.0926}$$

$$\boxed{\tau = 25.29 \text{ min}}$$

$$S = 0.0396 \text{ min}^{-1}$$

(2) A plug flow reactor ( $V=2\text{m}^3$ ) processes an aqueous feed (100 litre/min) containing reactant A ( $C_{A0} = 100 \text{ mol/litre}$ ). The reaction is reversible & represented by

$$A \rightleftharpoons R \quad -r_A = (0.04 \text{ min}^{-1}) C_A - (0.02 \text{ min}^{-1}) C_R$$

Find the equilibrium conversion & then find the actual conversion of A in the reactor.

Ans - For the PFR

$$\tau = \frac{C_{A0}}{r_A} \int_0^{x_A} \frac{dx_A}{(-r_A)} \quad (1)$$

As we know for the ~~first~~ order Rxn

$$\frac{k_1}{k_2} = \frac{m + x_e}{1 - x_e} \quad x_e = \text{EBM conversion}$$
$$m = \frac{C_{B0}}{C_{A0}}$$

$$\text{Here, } C_{B0} = 0 \Rightarrow m = 0$$

$$k_1 = 0.04 \text{ min}^{-1} \quad k_2 = 0.01 \text{ min}^{-1}$$

$$\therefore \frac{0.04}{0.01} = \frac{x_e}{1 - x_e} \Rightarrow x_e = 4 - 4x_e$$

$$\text{OR } x_e = \frac{4}{5} = 0.80$$

$$\boxed{x_e = 0.80}$$

NOW for actual conversion -

~~forward rxn~~ -

$$\cancel{-r_A = k_1 C_A - k_2 C_R}$$

$$\text{As } -r_A = k_1 C_A - k_2 C_R$$

$$C_A = C_{A0}(1 - x_A) \quad C_R = \cancel{C_{R0} + C_{A0}x_A}^0$$

$$-r_A = k_1 C_{A0}(1 - x_A) - k_2 C_{A0}x_A$$

Put it in eqn ①

$$\tau = \frac{1}{k_p} \int_0^{x_A} \frac{dx_A}{k_e(1-x_A) - k_2 x_A}$$

$$\tau = \int_0^{x_A} \frac{dx_A}{k_e(1-x_A) - k_2 x_A}$$

$$\tau = \frac{-1}{(k_p+k_2)} \int \frac{dt}{t}$$

$$\tau = - \left( \ln \left( k_p - (k_p+k_2)x_A \right) \right)_0^{x_A} \times \frac{1}{k_p+k_2}$$

$$\tau = \frac{-1}{(k_p+k_2)} \left( \ln \left( k_p - (k_p+k_2)x_A \right) - \ln(k_p) \right)$$

$$\therefore \tau = \frac{-1}{(k_p+k_2)} \left( \ln \left( \frac{k_p - (k_p+k_2)x_A}{k_p} \right) \right) \quad \text{--- ②}$$

$$\therefore \text{For PFR, } \tau = \frac{V x_{Ae}}{F_{Ae}} = \frac{2m^3 \times 100 \times 10^{-3} \text{ maf}}{200 \text{ lpt}} \times \frac{1000 \text{ lpt}}{1000 \text{ maf}}$$

$$\tau = \frac{V}{V_0} = \frac{2m^3}{200 \text{ lpt}} \text{ maf}$$

$$1m^3 = 1000 \text{ lpt}$$

$$\tau = \frac{2 \times 1000 \text{ lpt maf}}{200 \text{ lpt}}$$

$$= \frac{20 \text{ maf}}{\text{--- ③}}$$

$$\begin{aligned} & k_p(1-x_A) - k_2 x_A \\ &= k_p - k_p x_A - k_2 x_A \\ &= k_p - (k_p+k_2)x_A = 0 \\ & -(k_p+k_2)dx_A = dt \\ & dx_A = \frac{-1}{(k_p+k_2)} dt \end{aligned}$$

From eqn ② & ③

$$20 = \frac{-1}{0.04 + 0.02} \ln \left( \frac{0.04 - (0.04 + 0.02)x_A}{0.04} \right)$$

$$20 = \frac{-1}{0.06} \ln \left( \frac{4 - 5x_A}{4} \right)$$

$$\cancel{-2} - 2 = \ln(4 - 5x_A) - \ln 4$$

$$\cancel{-2} 0.386 = \ln(4 - 5x_A)$$

$$4 - 5x_A = e^{0.386} = 1.47$$

$$\frac{2.53}{5} = x_A$$

$$\boxed{\therefore x_A = 0.506}$$

~~Lect 1 (20)~~

## single Rxn:

→ only one rate law is written for single Rxn.

①

Batch reactor

$$t = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)}$$

PFR

$$\tau = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)}$$

- volume required for the same conversion will be same in both batch & PFR.

② CSTR & PFR

CSTR → Back mixing is allowed -  
composition is same inside the reactor & output.

PFR → Back mixing is not allowed

• Each & every molecules spending some time in PFR. (flat velocity profile)

CSTR

PFR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{x_A}{(-r_A)}$$

$$\frac{\tau}{C_{A0}} = \frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{(-r_A)}$$

$$\text{As } C_A = \frac{C_{A0}(1 - x_A)}{(1 + \varepsilon_A x_A)} \rightarrow \text{VURS}$$

$$\tau_m = \left( \frac{C_{A0} V}{F_{A0}} \right)_m = \frac{C_{A0} x_A}{-r_A} = \frac{C_{A0} x_A}{K C_A^n}$$

$$\text{As } C_A = \frac{C_{A0}(1 - x_A)}{(1 + \varepsilon_A x_A)}$$

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

$$\therefore \boxed{\tau_m C_{A0}^{n-1} = \frac{x_A (1 + \varepsilon_A x_A)^n}{K (1 - x_A)^n}} \rightarrow \begin{array}{l} \text{for CSTR} \\ \rightarrow \text{Nth order rxn} \end{array} \quad (2)$$

For PFR

$$\tau_P = \left( \frac{C_{A0} V}{F_{A0}} \right)_P = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)} = C_{A0} \int_0^{x_A} \frac{dx_A}{(K C_A)^n}$$

$$\therefore \tau_P = \left( \frac{C_{A0} V}{F_{A0}} \right)_P = C_{A0} \int_0^{x_A} \frac{(1 + \varepsilon_A x_A)^n dx_A}{K C_{A0}^n (1 - x_A)^n}$$

Now,

→ For PFR

$$\frac{\tau_m C_{A0}^{n+1}}{(\tau_p C_{A0}^{n+1})_p} = \left( \frac{C_{A0}^n V}{F_{A0}} \right)_p = \frac{1}{K} \int_0^{x_n} \frac{(1+\epsilon_n x_n)^n}{(1-x_n)^n} dx_n$$

divide the eqn of MFR by PFR (or  $\frac{\text{eqn 2}}{\text{eqn 1}}$ )

$$\frac{(\tau_m C_{A0}^{n+1})_m}{(\tau_p C_{A0}^{n+1})_p} = \frac{(C_{A0}^n V / F_{A0})_m}{(C_{A0}^n V / F_{A0})_p} = \frac{x_n (1+\epsilon_n x_n)^n / (1-x_n)^n}{\left[ \int_0^{x_n} \frac{(1+\epsilon_n x_n)^n}{(1-x_n)^n} dx_n \right]}$$

Now, for constant volume/density system,  
 $\epsilon_A = 0$

$$\Rightarrow \frac{(\tau_m C_{A0}^{n+1})_m}{(\tau_p C_{A0}^{n+1})_p} = \frac{\tau_m}{\tau_p} = \frac{(x_n / (1-x_n)^n)_m}{((1-x_n)^{n+1}-1)_p} \quad (n \neq 1)$$

using this we can comment,  
which reactor will have more volume.

① First order constant density system  
 $(\epsilon_A = 0)$

(n=1)

$$\frac{(C_{A0}^n V / F_{A0})_m}{(C_{A0}^n V / F_{A0})_p} = \frac{(\tau_m C_{A0}^{n+1})_m}{(\tau_p C_{A0}^{n+1})_p} = \frac{\tau_m}{\tau_p} = \frac{(x_n / (1-x_n))_m}{(-\ln(1-x_n))_p}$$

For second order constant density system ( $\epsilon_m = 0$ ) ( $n=2$ )

$$\frac{(\overline{C_{A_0}^n V/F_{A_0}})_m}{(\overline{C_{A_0}^n V/F_{A_0}})_p} = \frac{(\overline{\epsilon_m C_{A_0}^{n-1}})_m}{(\overline{\epsilon_p C_{A_0}^{n-1}})_p} = \frac{\overline{\epsilon_m}}{\overline{\epsilon_p}} = \frac{(x_n/(1-x_n))^2}{(x_n/(1-x_n))}^m_p$$

plot a graph of —

$$\frac{(\overline{C_{A_0}^n V/F_{A_0}})_m}{(\overline{C_{A_0}^n V/F_{A_0}})_p} = \frac{(\overline{\epsilon_m C_{A_0}^{n-1}})_m}{(\overline{\epsilon_p C_{A_0}^{n-1}})_p} \text{ vs } (1-x_n)$$

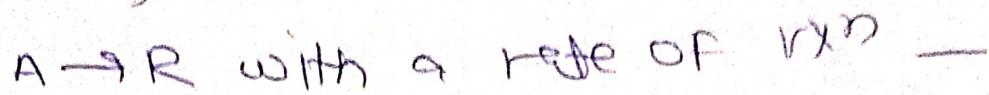
→ For identical feed rate & feed composition, the ordinate gives directly volume ratio of MFR & PFR as —

$$\left( \frac{V_m}{V_p} \right) \text{ vs } (1-x_n)$$

- For any given duty i.e. for given any specified composition for all positive reaction orders, the size of MFR is always larger than PFR.
- For low level of conversion, the reactor performance is slightly affected by flow type.

• Density variation during the reaction affects the design.

① Consider a first-order Rxn of constant density reaction →



$$-r_A = -\frac{1}{V} \frac{dN_A}{dt} = k C_A$$

② CSTR performance eqn -

$$\tau_m = \frac{U_m}{V_0} = \frac{C_{A0} r_A}{-r_A} = \frac{C_{A0} r_A}{K C_{A0} (1 - x_A)}$$

$$\therefore \boxed{K \left( \frac{U_m}{V_0} \right) = \frac{x_A}{1 - x_A}}$$

$$\therefore \boxed{x_A = \frac{K \left( \frac{U_m}{V_0} \right)}{1 + K \left( \frac{U_m}{V_0} \right)}}$$

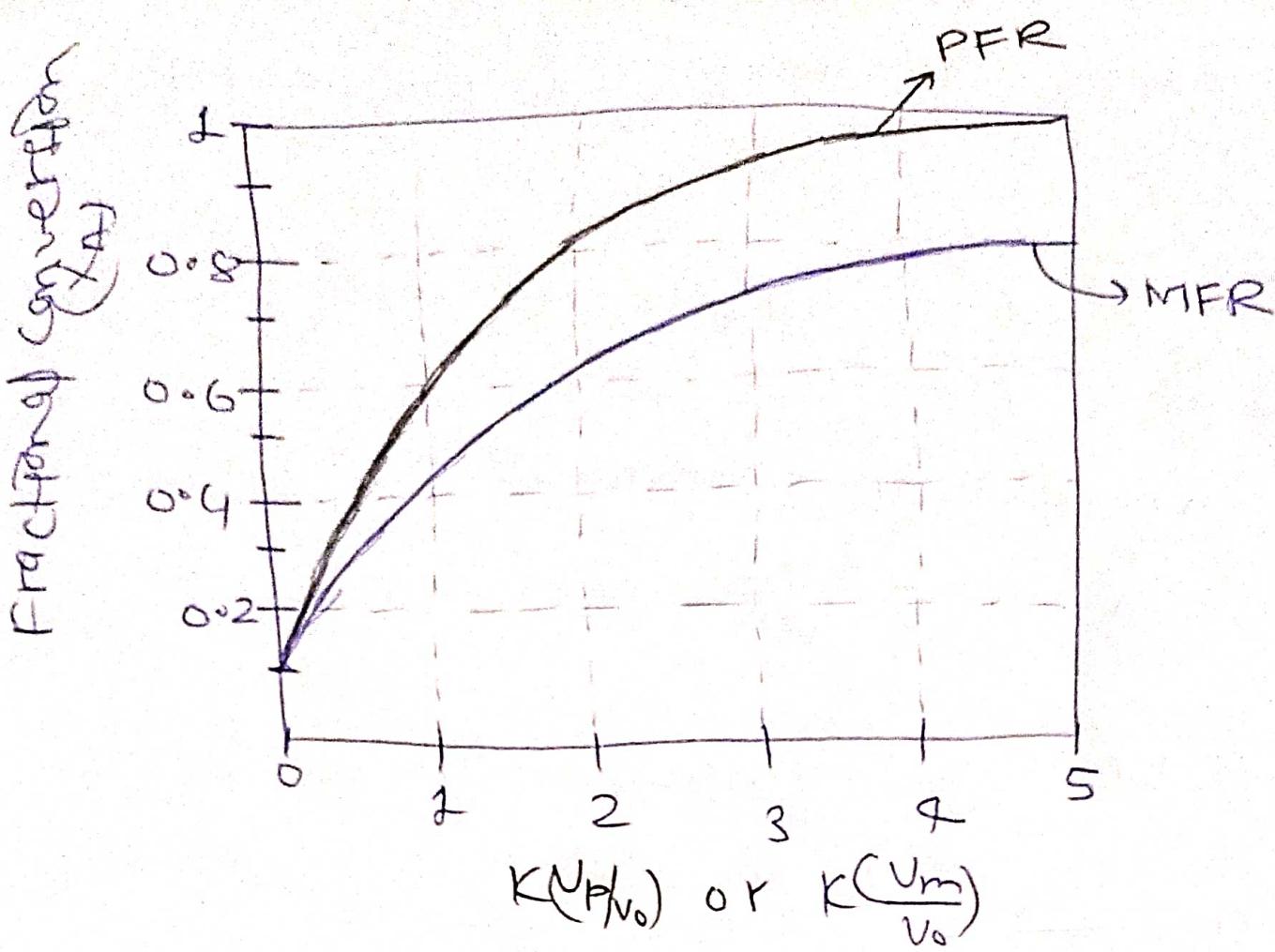
③ For PFR performance eqn -

$$\tau_p = \frac{V_p}{V_0} = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)} = x_{A0} \int_0^{x_A} \frac{r_A dx_A}{K C_{A0} (1 - x_A)}$$

$$\boxed{-K \left( \frac{U_p}{V_0} \right) = \ln (1 - x_A)}$$

$$\therefore \boxed{x_A = 1 - e^{-K \left( \frac{U_p}{V_0} \right)}}$$

$V_p$  = volume of  
 $V_0$  = volumetric  
flow rate  
of feed.



- For any specified conversion level, the volume of mixed flow reactor (MFR or CSTR) is larger than PFR.
- For a given space time, the conversion in plug flow reactor is higher than mixed flow reactor.

