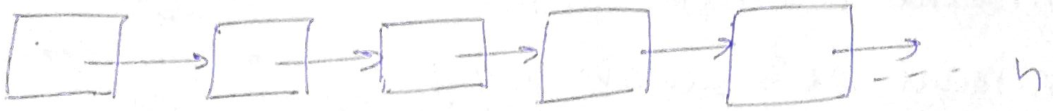
Q1)

a)

In − out + gen = Acc

{general (mass balance equation}
(& energy)



{for a train with no of 'n' compartments}
{our system}

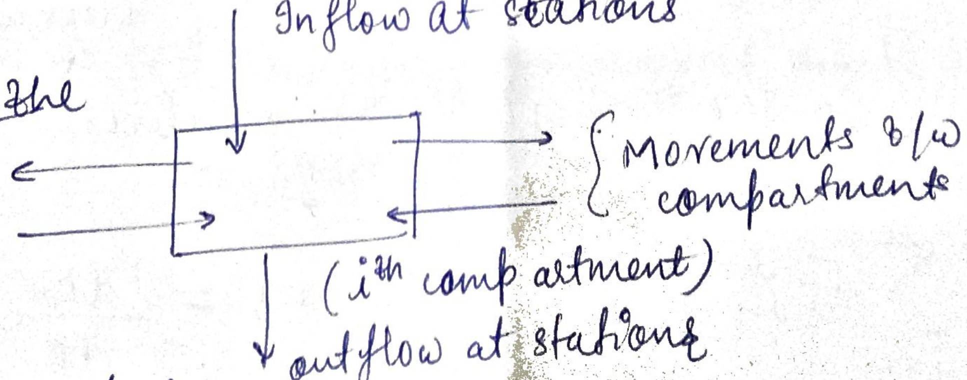
we can take a single compartment & treat it as our subsystem

- we treat (our trains) as connected compartment where people are equally likely to move or board the train.

- We assume there is no "ticket wise" differentiation b/w compartments.

- This brings uniformity of movement in trains compartments

Take A single ~~compartment~~ as the subsystem



Let $F(i, i+1)$ denote inflow to (i) from $(i+1)$

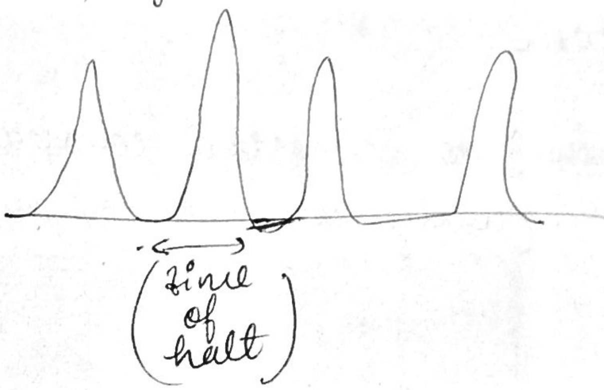
Inflow or movement majorly depends on the relative capacities of the train

$$F(i, i+1) = K(n_{i+1} - n_i)$$

we assume linear relation for movement {or inflow b/w compartment}

- Account for + for increasing & - ve for decreasing populations. {K be the proportionality constant}

Let $(F_{i,j})$ be the inflow at the j th station



Let there be (n) stations during the journey.

so during the journey total inflow

$$= \sum_{j=1}^{n} F_{i,j} \quad \forall\, t > t_j$$ { t_j time its stops at the j th stations }

So the single (i^{th}) compartment

$$\boxed{\sum_{\substack{j=1 \\ \forall t>t_j}}^{n} F_{i,j} + F(i, i+1) + F(i, i-1) = \frac{dN_i}{dt}}$$

N_i = no of passengers in the i^{th} compartment at any given time k will depend ~~@~~ upon relative capacity of compartment

as $N_i \rightarrow N_{max}$ {max passengers in the given compartment}

$k \longrightarrow k_0$ {max value of k

$$K \begin{cases} 0 & n_i < n_{max} \\ K & n_i > n_{max} \end{cases}$$

$$\sum_{j=1}^{n} F_{i,j} + F(i, i+1) + F(i, i-1) = \frac{dN_i}{dt}$$

$$\hookrightarrow \sum_{j=1}^{n} F_{i,j} + K(n_{i+1} - n_i) + K(n_{i-1} - n_i) = \text{"}$$

$$\hookrightarrow \sum_{j=1}^{n} F_{i,j} + K(n_{i+1} + n_{i-1} - 2n_i) = \frac{dn_i}{dt}$$

n (unknown)

4 unknowns

Assuming we have all passengers info about boarding the trains or {passengers chart} we can elimanate the (n) unknowns

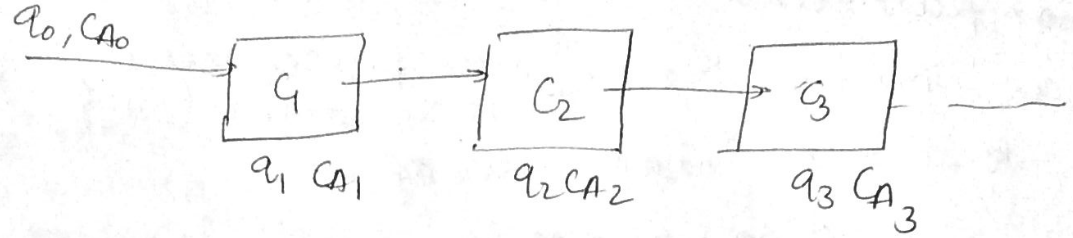
so only k, n_{i+1}, n_{i-1}, n_i are the remain unknowns

If we unsteady state.

4 unknown 1 mass balance

$$\boxed{4 - 1 = 3 \text{(DOF)}}$$

For tanks in series



for the i^{th} tank
using
$\dot{In} - \dot{Out} + \dot{Gen} = \dot{Acc}$

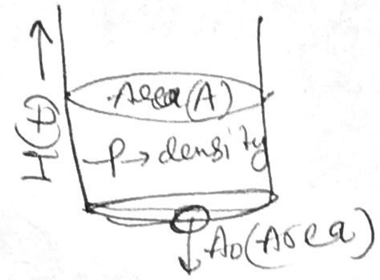
$$q_{i-1} C_{Ai-1} - q_i C_{Ai} - k C_{Ai} V = \frac{V\, dC_{Ai}}{dt}$$

$V =$ vol^m of tank

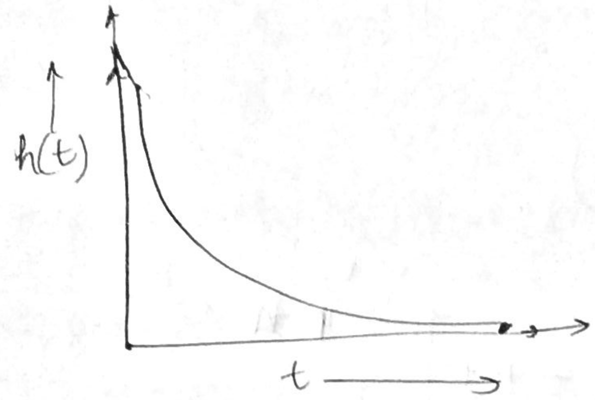
Comparison

- train has bidirectional movement but tanks have single direction movement
- trains compartment also has inflow & outflow ~~out the~~ outside the system but reactor has out movement b/w compartments
- Both ~~are~~ have relatively same equations for mass balance.

Q) 2



a)



h(t) is decreasing function of time can't be linear because height drops ~~faster~~ slower as the liquid empty the bottle initially it decrease faster than it slows down to zero eventually

b) Assuming incompressible liquid

$(AV_1 = A_0 V_2)$ → principle of continuity surface

V_1 & V_2 are velocity of liquid at the 2 crosssections

$q = Kh^n$

(can't be constant as height would decrease linearly)

So it ~~is~~ seems a reasonable approximation

$n \neq 1$

because height decrease exponentially & take inf time to complete which is not the case in realworld.

$$-A\frac{dh}{dt} = k_1 h^n$$

$$\frac{dh}{dt} = k_1 h^n \quad \text{let} \left(\frac{k_1}{A} = k\right)$$

$$\int_{h_0}^{h(t)} \frac{dh}{h^n} = -\int_0^t k\,dt$$

$$\left(\frac{h^{-n+1}}{1-n}\right)_{h_0}^{h} = -(kt)$$

$$h = \left((1-n)\left[\frac{h_0^{1-n}}{1-n} - kt\right]\right)^{1/1-n}$$

for both $n>1$ & $n<1$

h will decrease with time

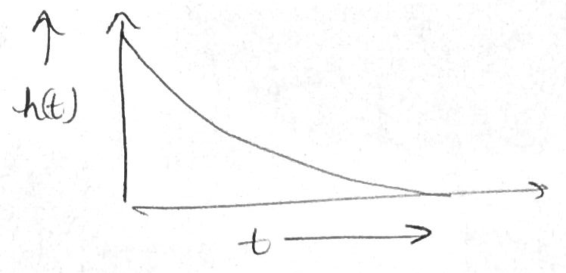
so will have to check differential equation

$$\left(\frac{1}{h}\right)\frac{dh}{dt} = \cancel{\frac{-1}{(n-1)}}\left(\frac{1}{1-n}\right)^2\left(\frac{1}{\left[\frac{h_0^{1-n}}{(n-1)} + \frac{kt}{\cancel{A}}\right]}\right)\cdot\frac{(n-1)k}{A}$$

{in class solved}

$n \cancel{<} 1$ for increasing t slope is decreasing

$\therefore$ ~~(...)~~ $n < 1$



for no viscocity {using dimensional analysis)

$q = \frac{L^3}{T}$. $A_0 = L^2$

$h = L$ $\quad g = L/T^2$

4 {unknown} − 2 {dimen} = 2

2 groups are formed

it canbe formed in many ways

{ possible ways { shown in class} }

$\left(\frac{A_0}{h^2}\right) \quad \left(\frac{q^2}{gA_0^2 h}\right)$

$f\left(\frac{A_0}{h^2}\right) = \left(\frac{q^2}{gA_0^2 h}\right)$ → canbe expressed as a function

as $\frac{A_0}{h^2} \longrightarrow$ or $A_0 \longrightarrow 0$ small hole

$f(0) \longrightarrow$ const^n

$\frac{q^2}{gA_0^2 h} = c$

$q = \sqrt{cgA_0^2}\,(h)^{1/2}$

$q \propto (h)^{1/2}$

for visocity

unknown = ρ, μ, g, A_0, h, q

graphs $6-3=3$

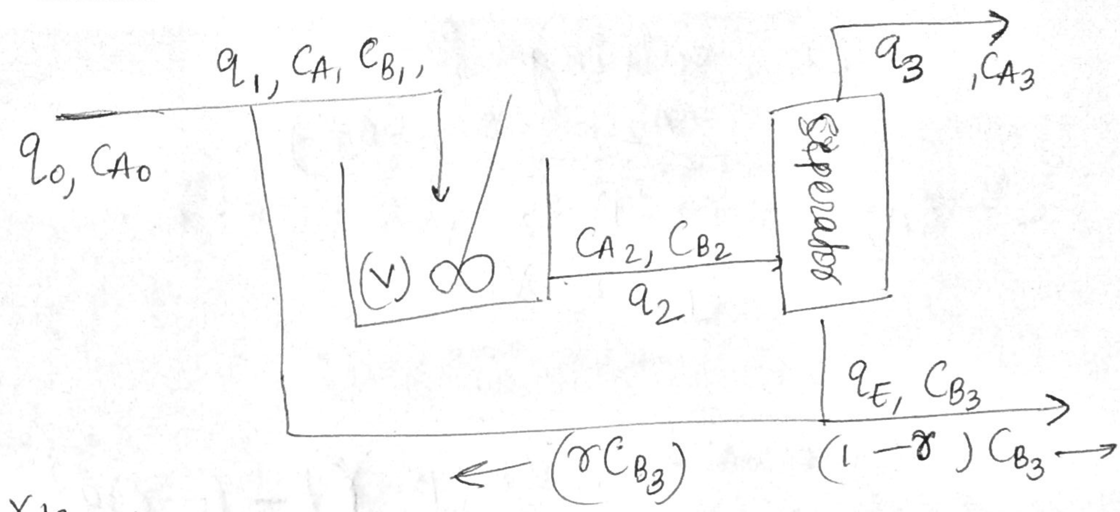
$$\mu = \frac{ML}{T}, \quad \rho = \frac{M}{L^3}$$

possible groups {discussed in class}

$$\frac{\rho q}{\mu h}, \frac{\rho q}{\mu \sqrt{A}}, \frac{q^2}{g A_0^2 h}$$

$$f\left(\frac{A_0^2}{h}, \frac{\rho q}{\mu\sqrt{A_0}}\right) = \frac{q^2}{g A_0^2 h}$$

Q) 3



Rxn

$$A + \beta B \longrightarrow \gamma \beta + \text{Pdts}$$

$(\gamma > \beta)$

unknown, $C_{A_0}, C_{A_1}, C_{A_2}, C_{A_3}$ (concn of A)

$C_{B_1}, C_{B_2}, C_{B_3}$ (concn of B), V, q_1, q_2, q_E, q_3 (flow rates), γ {recycler fraction}

given, $\longrightarrow$ $C_{A_1}, V, q_1, q_2, \gamma$

rate $=$ $\underline{r_A = k\, C_A C_B}$

BALANCE Equation

$$C_{A_1} q_1 - q_2 C_{A_2} - k\, C_{A_2} C_{B_2} V = 0 \longleftrightarrow (1)$$

$$q_2 B_2 = q_E C_{B_3} \longrightarrow (2)$$

$$(q_2 = q_E + q_3) \longrightarrow (3)$$

$$q_2 C_{A_2} = q_3 C_{A_3} \longrightarrow (4)$$

$$C_{B_1} q_1 - q_2 C_{B_2} - k C_{A_2} C_{B_2} \beta + k C_{A_2} B_2 \gamma = 0 \longrightarrow (5)$$

$$q_1 B_1 = \gamma q_2 C_{B_2} \longrightarrow (6)$$

On solving for C_{A2}, C_{B2}, C_{B3}

$$C_{A2} = \frac{(\gamma-1)}{(\beta-\gamma)}\left(\frac{q_2}{VK}\right)$$

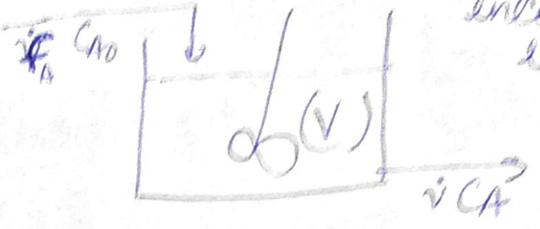
$$C_{B2} = \frac{C_{A1} q_1 VK(\beta-\gamma) - (1-\gamma)q_2^2}{KV q_2^2(1-\gamma)}$$

$$C_{B3} = \left(\frac{q_2}{q_E}\right) C_{B2} = \frac{C_{A1} q_1(\beta-\gamma)VK - (1-\gamma)q_2^2}{KV q_2^2(1-\gamma)q_E}$$

Q) 4   A - pdtq

incompressible liq {v is = const}

(CSTR)



So Assuming

- V = constant
- well mixed tank {conc^n is same throughout}

$\dot{F}_A$ = flowmetric flowrate

C_A = conc^n in the tank at time (t)

$\dot{In} - \dot{out} + Gen = \dot{Acc}$

$\{-r_A = KC_A\}$ following the rate law

$m_{in} - m_{out} + (-r_A) = \left(\frac{dm}{dt}\right)$
↳ {mass}

~~Fin CAin - Fout~~ $F_{in} C_{Ain} - F_{out} C_{Aout} + K C_{Aout} = \frac{d(\rho V)}{dt}$

For the rate law

$r_A = -KC_A$

$\tau_{rxn} = 1/K$ τ_{rxn} = (time of rxn)

$\tau_n = \left(\frac{V}{F}\right)$ V = Vol^m
F = flowrate

↳ (residence time)

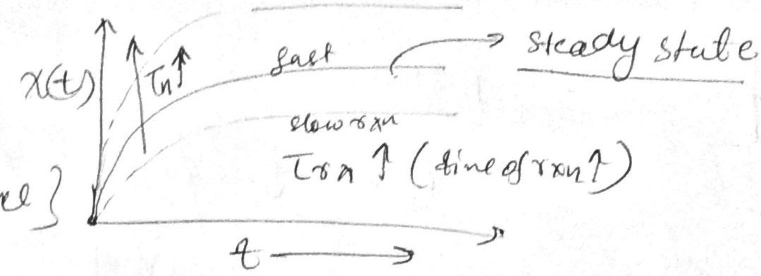
$C_A = C_{A0}(1 - x(t))$

x(t) is conversion rate

Time scales

$\tau_{rxn} = 1/k$ {residence time}

$\tau_n = V/F$ {rxn time}



$$\dot{In} - \dot{Out} + \dot{Gen} = \dot{Acc}$$

$$F C_{A0} - F C_A - k C_A V = V\left(\frac{dC_A}{dt}\right)$$

$$F\left(C_{A0} - C_{A0}(1 - x(t))\right) - kV C_{A0}(1 - x(t)) = V\frac{dC_A}{dt}$$

$$F C_{A0}(x(t)) - kV C_{A0}(1 - x(t)) = V\frac{dC_A}{dt}$$

$$x(t) - k(V/F)(1 - x(t)) = (V/F)\frac{dx(t)}{dt}$$

$$x - \frac{(V/F)}{(1/k)}(1 - x) = (V/F)\frac{dx}{dt}$$

$$x - \left(\frac{\tau_n}{\tau_{xn}}\right)(1 - x) = \tau_n\frac{dx}{dt}$$

$$\frac{\tau_n}{\tau_{rxn}} - x\left(\frac{\tau_n}{\tau_{rxn}} + 1\right) = \tau_n\left(\frac{dx}{dt}\right)$$

$$\int_0^t dt = \int_0^x \frac{\tau_n \, dx}{\frac{\tau_n}{\tau_{rxn}} - x\left(\frac{\tau_n}{\tau_{rxn}} + 1\right)}$$

$$\int_0^t dt = \int_0^x \frac{dx}{\beta - \alpha x} \qquad \beta = \left(1/\tau_{xn}\right)$$

$$\alpha = \left(\frac{1}{\tau_{xn}} + \frac{1}{\tau_n}\right)$$

$$t = \left[-\frac{1}{\alpha} \ln(\beta - \alpha x) \right]_0^x$$

$$t = +\frac{1}{\alpha} \ln\left(\frac{\beta}{\beta - \alpha x} \right)$$

on simpifying

$$x = \frac{\beta}{\alpha} \left(1 - \exp(-\alpha t) \right)$$

$$x = \frac{1}{\left(1 + \frac{\tau_{rxn}}{\tau_n}\right)} \left(1 - \exp\left[-t \left(\frac{1}{\tau_{xn}} + \frac{1}{\tau_n} \right) \right] \right)$$

$$x = \frac{1 - \exp\left\{ -t \left(\frac{1}{\tau_{rxn}} + \frac{1}{\tau_n} \right) \right\}}{(\tau_{rxn}) \left(\frac{1}{\tau_{xn}} + \frac{1}{\tau_n} \right)}$$ → like a 1^{st} order differential eqn's solution

$$\tau = \left(\frac{1}{\frac{1}{\tau_{xn}} + \frac{1}{\tau_n}} \right)$$

→ timescale or time constant

$\tau_n \uparrow \Rightarrow$ more time of residence {or time to react}

If $\tau_{rxn} \uparrow \Rightarrow$ conversion is lesser

τ_{xn} is generally not controlled cause it is decided by the rxn

{(τ_n) can be controlled by controlling flow rate}

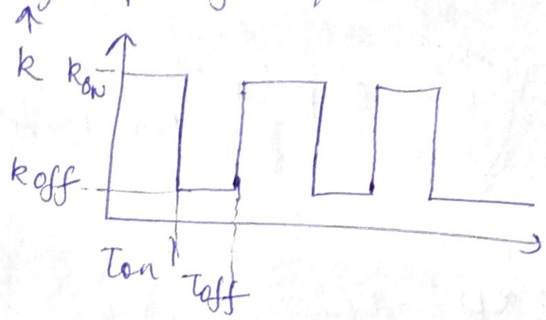
Q) 5

$$A + B \xrightarrow{K} C$$

for light on $\cdot$ $r = K_{ON} C_A C_B$

for — off $r = K_{off} C_A C_B$

so graph of K v/s t



- for light on

$$r_A = \frac{dC_A}{dt} = K_{ON} C_{A0}(1-x)(C_{B0} - C_{A0}x)$$

x is conversion factor

$$\frac{dx}{dt} = C_{A0}K_{ON}(1-x)\left(\frac{C_{B0}}{C_{A0}} - x\right) \qquad \alpha = \left(\frac{C_{B0}}{C_{A0}}\right)$$

$$= K_{ON}(1-x)(\alpha - x)$$

$$\int_0^x \frac{dx}{(1-x)(\alpha-x)} = C_{A0}K_{ON}\int_0^{t_{on}} dt$$

$$\frac{1}{(\alpha-1)}\left(\int_0^x \left(\frac{1}{1-x} - \frac{1}{(\alpha-x)}\right) dx\right) = K_{ON}C_{A0}\int_0^{T_{ON}} dt$$

$$\frac{1}{\alpha-1}\left[\ln\left(\frac{1-x}{\alpha-x}\right)\right]_0^x = (K_{ON} C_{A0} T_{ON})$$

$$T_{ON} = \frac{1}{K_{ON} C_{A0} (\alpha - 1)} \ln \left[\frac{\alpha - x}{\alpha (1 - x)} \right]$$

Now conversion = Y

$$r = K_{off} C_A C_B \qquad C_{new} = C_{A0}(1-x)$$

$$\left(\frac{dC_A}{dt}\right) = K_{off} C_{A_{new}} (1 - Y) \left(C_{B_{new}} - C_{A0} x - C_{A_{new}} Y \right)$$

$$\frac{dY}{dt} = K_{off} C_{A0}(1-x)(1-y) \left(\frac{C_{B0} - C_{A0} x}{C_{A0}(1-x)} - y \right)$$

$$\frac{dy}{(1-y)\left(\frac{C_{B0} - C_{A0} x}{C_{A0}(1-x)} - y \right)} = \int_0 dt \left(K_{off} C_{A0} (1-x) \right)$$

Integration both sides

& simpifying for T_{off}

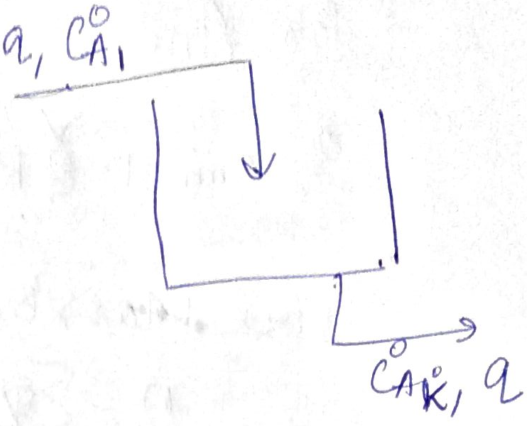
$$T_{off} = \frac{1}{(\alpha - 1)(C_{A0}(1-x))} \ln \left(\left(\frac{\alpha - Y}{\alpha - x} \right) \frac{(1-x)}{1-y} \right)$$

$$T_{total} = T_{ON} + T_{off} + T_{ON} + - T_{off}$$

→ using this result we can generalise for ~~other~~ next T_{on} & T_{off}

Q) 6

$$A_1 + A_1 \xrightarrow{k_1} A_2$$
$$A_2 + A_1 \xrightarrow{k_2} A_3$$
(CSTR) $$A_3 + A_1 \xrightarrow{k_3} A_4$$
$$\vdots$$
$$A_{m-1} + A_1 \xrightarrow{k_{m-1}} A_m$$



$k = 1, 2, 3 \ldots m$

given
$$k_i = \frac{k}{i} \;\forall\; (i = 1 \text{ to } m-1)$$

Mass balance on A_1

$$q C_{A_1} - q C_{A_1} \times (-k_1 C_{A_1}^2) - q C_{A_1}(-k_2 C_{A_2} A_1) - q C_{A_1}(-k_3 C_{A_3} A_1) \ldots = 0$$

$$\Rightarrow q C_{A_1} + q C_{A_1}(k_1 C_A^2 + k_2 C_{A_2} A_1 + k_3 C_{A_3} A_1 \ldots k_{m-1} C_{A_{m-1}} A_1) = 0$$

for A_2

$$q(k_1 C_{A_1}^2 - k_2 C_{A_1} C_{A_2}) = 0$$

for A_3

$$q(k_2 C_{A_2} C_{A_1} - k_3 C_{A_3} A_1) = 0$$

so Generalise equation $\forall$ m = 2 to m-1

$$q\left\{k_{m-1} C_{A_{m-1}} C_{A_1} - k_m C_{A_m} C_{A_1}\right\} - q C_{A_m} = 0$$

for m = 1

for A_m

$$-qC_{A_m} + \cancel{q}V k_{m-1} C_{A_1} C_{A_{m-1}} = 0$$

Total Mass balance

$$\underline{m = \sum q C_{Ai} \times M_i} \rightarrow \left(\begin{array}{l}M_i \text{ is the} \\ \text{molar mass}\end{array}\right)$$

$$= \underbrace{q\left(C_{A_1} M_1 + C_{A_2} M_2 + C_{A_3} M_3 \text{ --- }\right)}_{\text{mass exiting from system}}$$

for overall mass

$$\cancel{q} C_{A_1}^{0} M_1 = \cancel{q}\left(C_{A_1} M_1 + C_{A_2} M_2 + C_{A_3} M_3 \text{ --- }\right.$$

$$M_1/M_1 = 1 \quad \frac{M_2}{M_1} = 2, \quad \frac{M_3}{M_1} = 3 \text{ --- }$$

$$C_{Ai}^{0} = C_{A_1} + 2C_{A_2} + 3C_{A_3} \text{ --- }$$

$$C_{Ai}^{0} = \sum_{j=1}^{m-1} j\, C_{Aj}$$

$$C_{Am} = \underline{k_{m-1} C_{A_1} C_{Am-1}}$$

$$C_{Am} = \frac{q k_{m-1} C_{Am-1} C_{A_1}}{q k_m C_{A_1} + q}$$

Assuming $\boxed{\eta = \left(\frac{kV}{q}\right)}$

$$\frac{V\cancel{K}_{m-1}}{\cancel{Q}\ldots} \quad \cancel{\frac{\frac{C_{Am-1}}{C_{A1}^{0}} \frac{C_{A1}}{C_{A0}}}{\left(\frac{C_{A1}}{C_{A10}^{2}} + q\right)}}$$

$$\frac{V K_{m-1} \left(\frac{C_{Am-1}}{C_{A0}}\right) \frac{C_{A1}}{C_{A0}}}{V K_m \frac{C_{A1}}{C_{A0}^2} + \frac{q}{C_{A0}^2}}$$

on simplifying & puting $K_i = \left(\frac{k}{q}\right)$

$$C_{Am} = \frac{\eta \left(\frac{C_{Am-1} C_{A1}}{m-1}\right)}{\frac{1}{C_{A0}^2}\left(1 + \frac{\eta C_{A1} C_{A0}}{m}\right)}$$

C_{A1} from 1st equation

$$C_{Am} = \frac{\left(\frac{C_{Am-1} C_{A1}}{\cancel{m-1}}\right)}{\frac{1}{C_{A0}^2}\left(\frac{1}{\eta} + \frac{C_{A1} C_{A0}}{m}\right)}$$

for case-1 $\eta <<< 1$ $\quad \frac{1}{\eta} >>>> \left(\frac{C_{A1} C_{A0}}{m}\right)$

$$\therefore \quad C_{Am} = \eta C_{A0} \left(\frac{C_{Am-1} C_{A1}}{m-1}\right)$$

case $n >>> 1$ $\quad \frac{1}{\eta} <<<< \left(\frac{C_{A1} C_{A0}}{m}\right)$

$$C_{Am} = \left(\frac{m}{m-1}\right)\frac{(C_{Am-1})}{C_{A0}^2}$$

$$\frac{C_{A1}}{C_{A0}} = \bar{C}_A$$

so the general form of equation

$$\bar{C}_A = \frac{\alpha}{(m-1)\left(\frac{1}{\eta} + \frac{\beta}{m}\right)}$$

when

$m \uparrow$ $\eta \uparrow$ for $\bar{C}_A$ to be constant

so greater value of m greater the value of η

$$\eta = \frac{KV}{q} = \left(\frac{V/q}{1/K}\right)$$

= ratio of time scale

so $\eta > 1$ mean

residence time > rxn time

& vice versa

Q) 7

$$A + B \longrightarrow AB$$

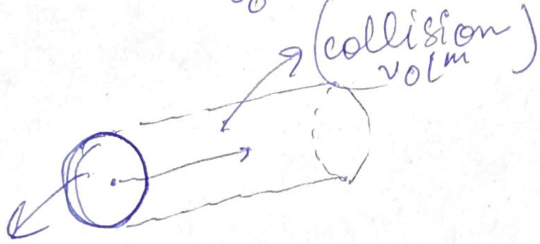
(gas phase elementary rxn)

$$r_A = (K C_A C_B)$$

A & B $\longrightarrow$ spherical molecules

rxn time $= \dfrac{1}{K C_{A0}}$ if A is limiting

" $= \dfrac{1}{K C_{B0}}$ if B is limiting



length scale = mean free path

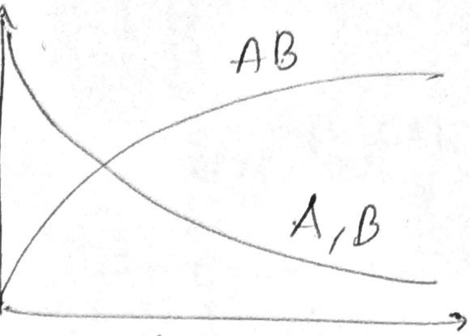
Mean free path = distance travelled by particle b/w successive collisions

** free path of spherical particles is clyindrical in shape

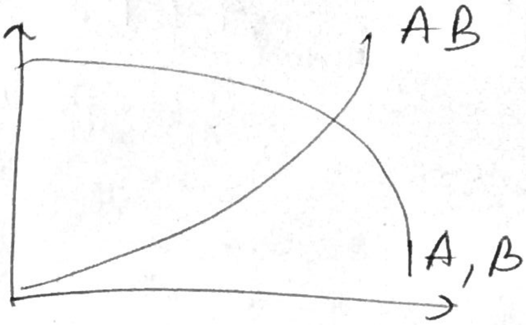
∴ the dia of vessel should be equal or greater than mean free path.

Dimensionless time = time ratio = $\dfrac{\text{time}}{\text{Timescale}}$

$$= \frac{t}{\left\{ \frac{1}{K C_{A0}} \text{ or } \frac{1}{K C_{B0}} \right\}}$$



fast



Slow