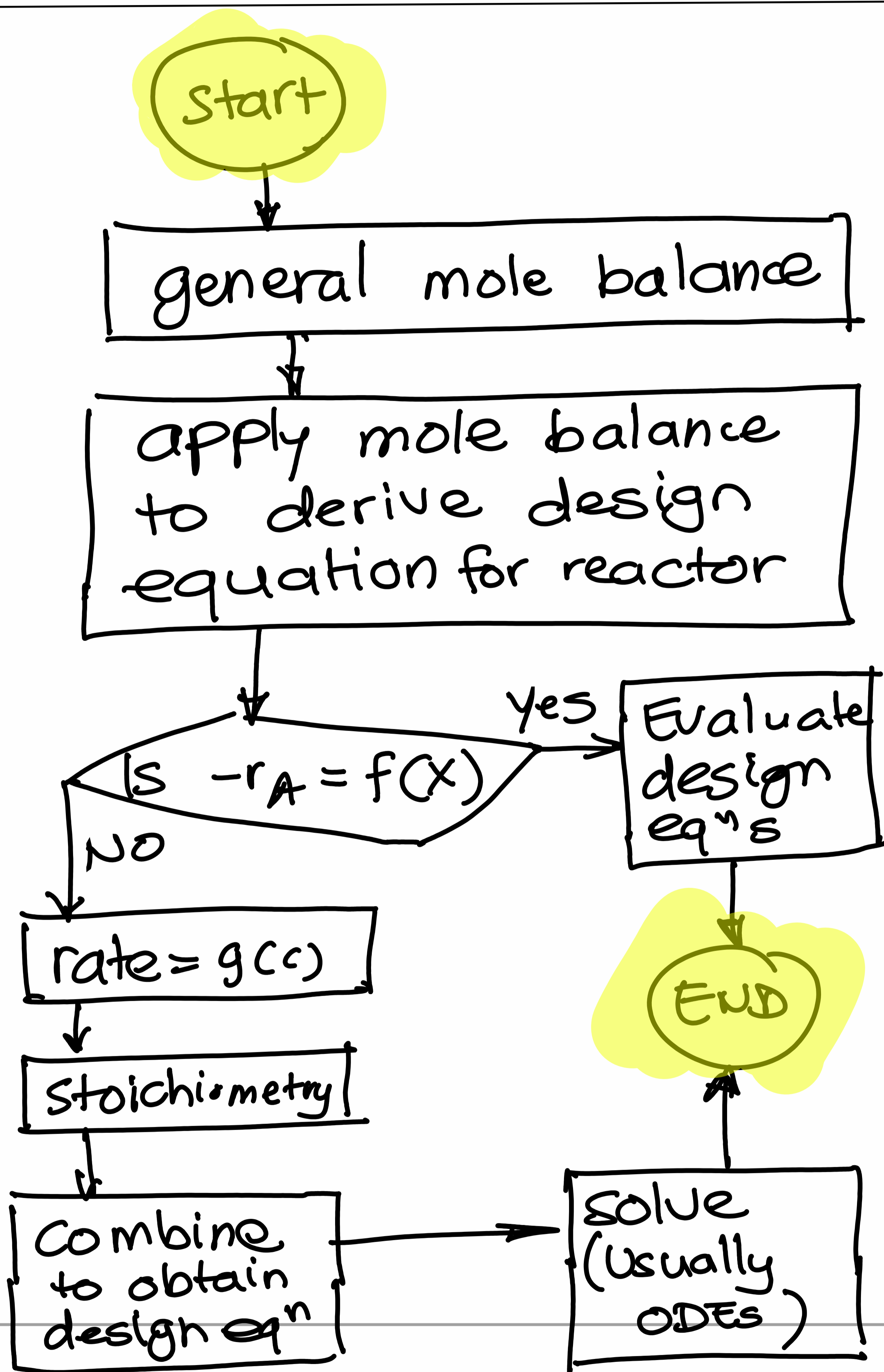


Notes on
chemical
Reaction
Engineering

Chapter 5

Isothermal reactor design

Design
Structure of
isothermal
reactors



⇒ Use algorithm rather than memorizing equations

The algorithm

① Mole balance

② rate law

③ stoichiometry

④ combine

⑤ evaluate

① Mole balance

$$F_{A0} - F_A + \int_V^V r_A dV = \frac{dN_A}{dt}$$

⇓ apply this to the specific reactor in question

In terms of X

• Batch reactor (ODE)

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

• CSTR (algebraic equation)

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

• PFR (ODE)

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

• PBR (ODE)

$$F_{A0} \frac{dX}{dW} = -r'_A$$

② Rate law

If $-r_A$ is given as $f(X)$
we can directly solve the
design equations otherwise
we need to convert
the rate expression and
make it a function of X

③ Stoichio- metry

If $-r_A \neq f(X)$

Say $-r_A = g(C)$ then
we need to use stoichiometry
and write the rate law
in terms of X

Liquid phase:

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

$$C_B = C_{A0}\left(\theta_B - \frac{b}{a}X\right)$$

Gas phase:

$$C_A = C_{A0} \frac{(1-X) P}{(1+\epsilon X) P_0} \quad (\text{const } T)$$

For PFRs: We also need to consider
pressure drop along the length

$$\frac{dP}{dW} = \frac{\alpha}{2P}(1-\epsilon X), \quad P = \frac{P_0}{1+\epsilon X}$$

④ Combine

Gathering all the equations

- mole balance
- rate law
- stoichiometry
- other eqⁿ: (like pressure drop)

gives us a system of equations we must solve to obtain reactor volume.

⑤ Evaluate/
solve

The system of equations obtained by combining can be solved

- analytically
- graphically
- numerically
- using software.

French Menu Analogy Choices

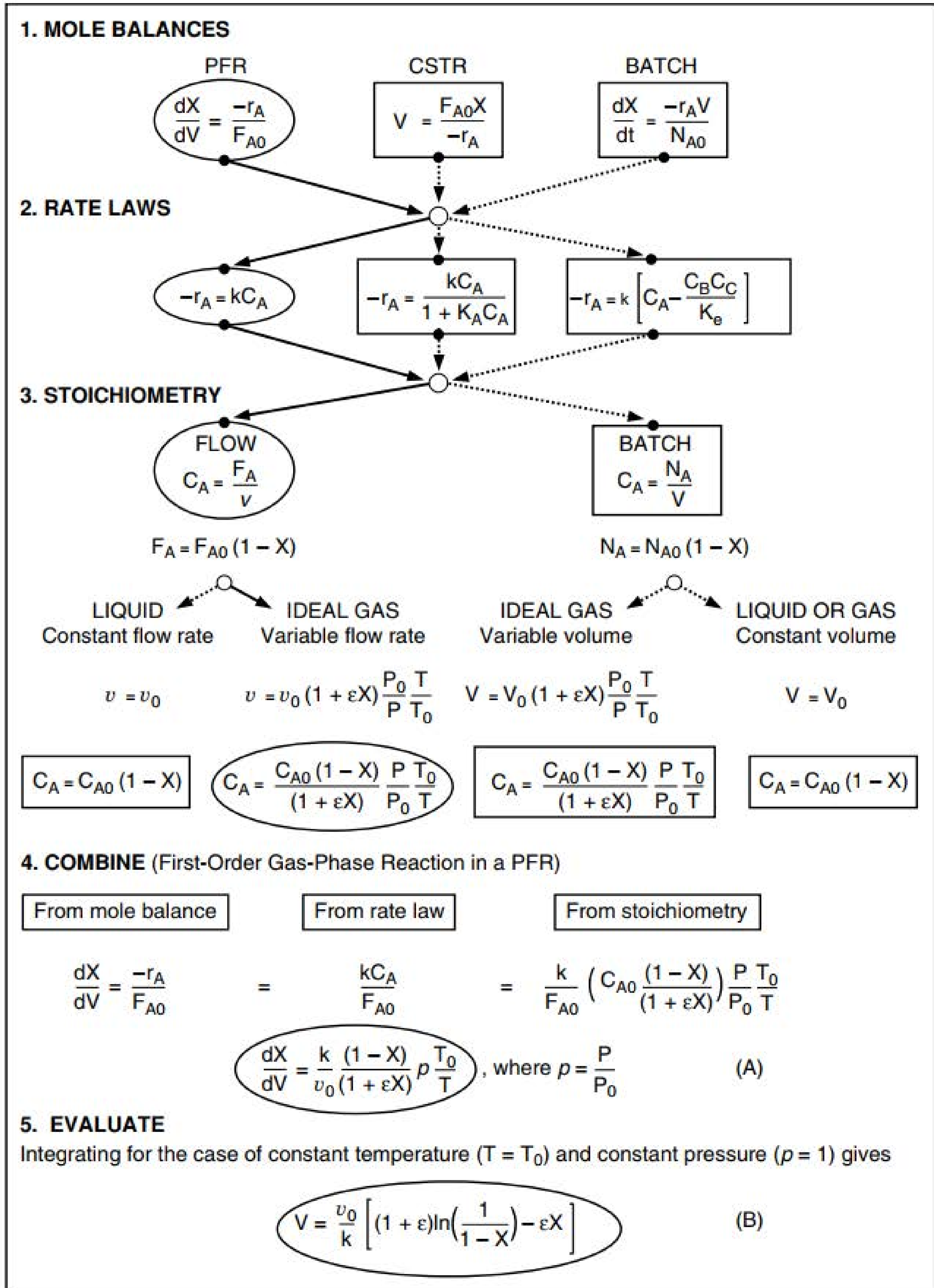


Figure 5-2 Algorithm for isothermal reactors.

Batch Reactor

⇒ Usually we are interested in calculating batch reaction time for a given X or X for a given batch reaction time.

$-r_A$ is now in terms of X

Consider rxn: $2A \rightarrow B + C$

Algorithm:

① Mole balance (const. $V = V_0$)

$$N_{A0} \frac{dX}{dt} = -r_A V_0$$

$$C_{A0} = \frac{N_{A0}}{V_0}$$

$$\therefore \frac{dX}{dt} = \frac{-r_A}{C_{A0}}$$

② rate law

$$-r_A = k_2 C_A^2$$

③ Stoichiometry

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

$$\therefore -r_A = k_2 C_{A0}^2 (1 - X)^2$$

④ Combine

$$\frac{dX}{dt} = k_2 C_{A0} (1 - X)^2$$

Evaluate ⇒ $t = \frac{1}{k_2 C_{A0}} \int_0^X \frac{dX}{(1 - X)^2}$

For 2nd order reaction

$$t = \frac{1}{k_2 C_{A0}} \frac{X}{1 - X}$$

Similarly for 1st order reaction we can show that

$$t = \frac{1}{k_1} \ln \left(\frac{1}{1-x} \right)$$

Batch reactor times

First order $k_1 (1/s)$	2 nd order $k_2 C_{A0} (1/s)$	Reaction time (t_R)
10^{-4}	10^{-3}	Hours
10^{-2}	10^{-1}	Minutes
1	10	Seconds
1000	10000	milliseconds

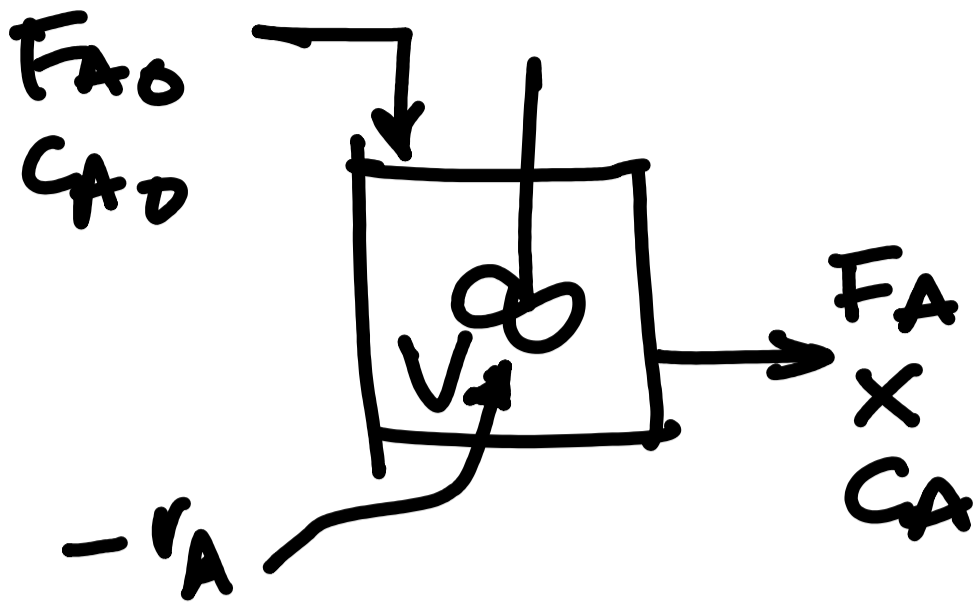
Batch cycle times

↳ Time between batches

Activity	Time (h)
1. charge feed t_f	0.5 - 2
2. heat to rxn temp t_e	0.5 - 2
3. reaction t_R	varies
4. Empty and clean reactor t_c	1.5 - 3.0
Total	$\Rightarrow (2.5h \text{ to } 7.0h) + t_R$

Batch reaction time is just one component in batch cycle time.

CSTR



Mole balance

$$V = \frac{F_{A0} X}{-r_A|_{\text{exit}}}$$

⇒ Concentration everywhere in the reactor is same as the exit concentration.

∴ rate everywhere = $-r_A|_{\text{exit}}$ in the reactor

Space time

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



time necessary to process one reactor volume of fluid based on inlet conditions.

$$F_{A0} = C_{A0} v_0$$

$$\therefore \frac{V}{v_0} = \tau = \frac{C_{A0} X}{-r_A|_{\text{exit}}}$$

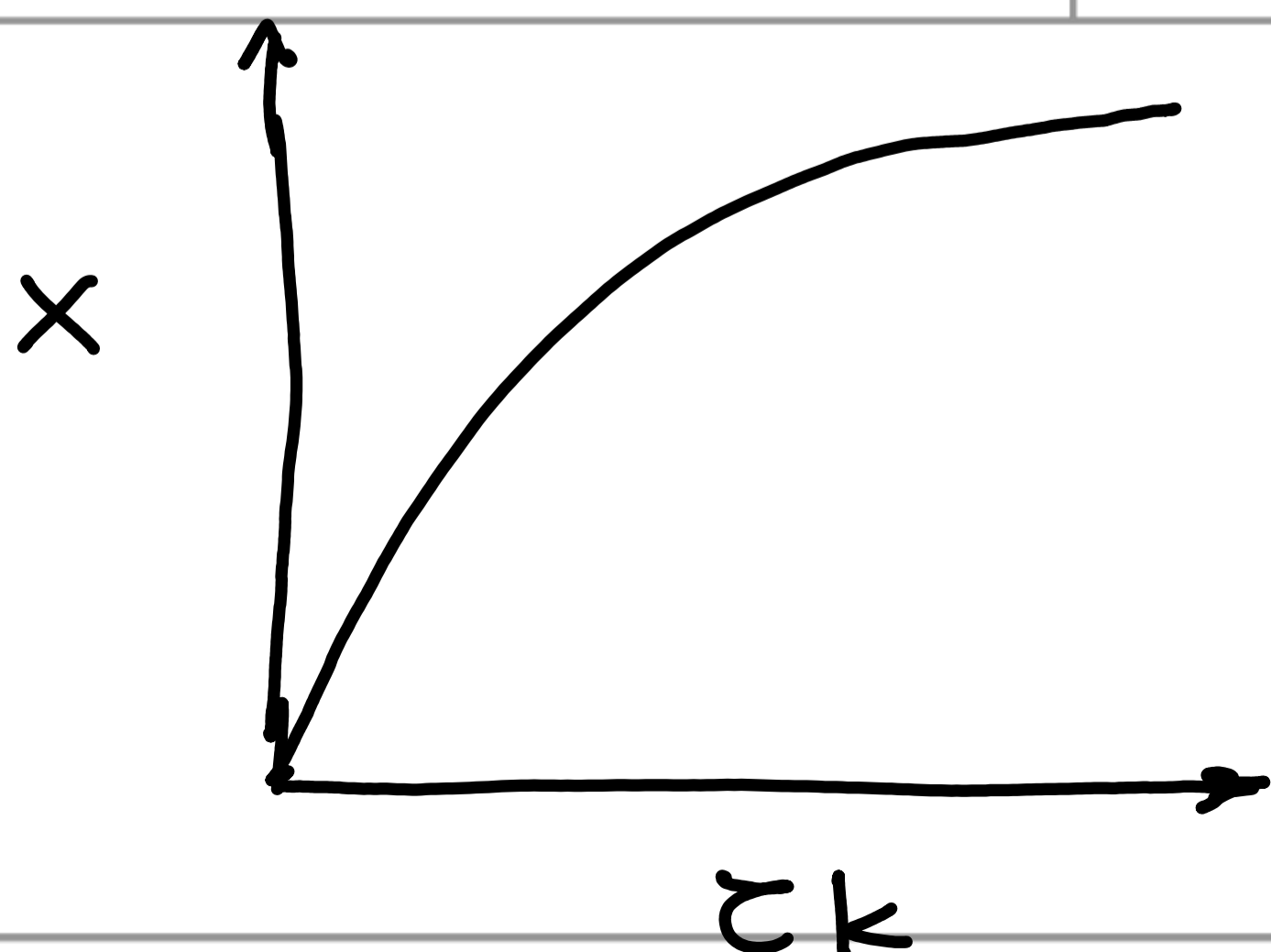
First order reaction:

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

$$\tau = \frac{1}{k} \frac{X}{1-X}$$

or

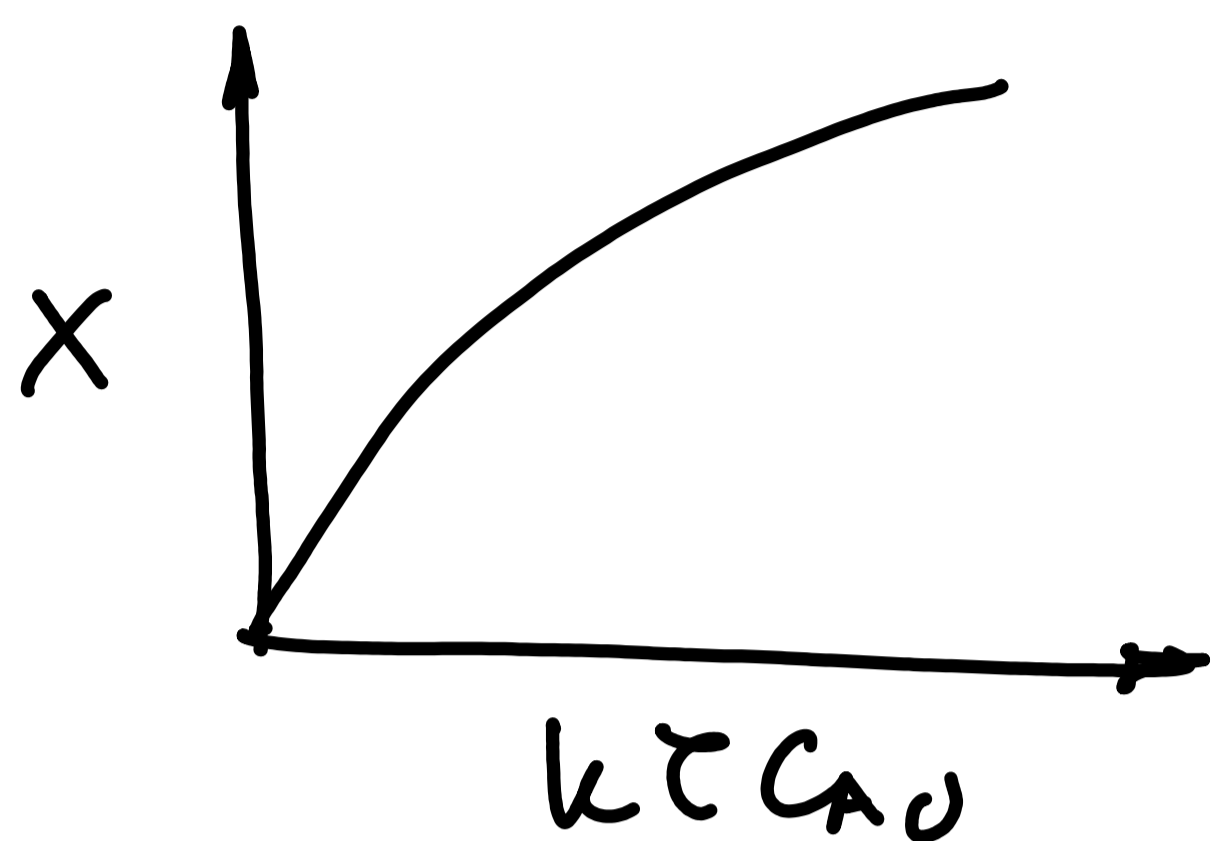
$$X = \frac{\tau k}{1 + \tau k}$$



⇒ Increasing τk increases X

- ↳ Increase temperature (k)
- ↳ Increase space time (τ)
 - ↳ Increase volume
 - ↳ decrease v_0

2nd order rxn
in CSTR



Damköhler No

$$Da = \frac{-r_{A0} V}{F_{A0}}$$

1st and 2nd
order Da

$$V = \frac{F_{A0} X}{k C_A^2} = \frac{v_0 C_{A0} X}{k C_{A0}^2 (1-X)^2}$$

$$\tau = \frac{X}{k C_{A0} (1-X)^2}$$

or

$$X = \frac{(1 + 2k\tau C_{A0}) - \sqrt{1 + 4k\tau C_{A0}}}{2k\tau C_{A0}}$$

Da gives quick estimate of degree of conversion that can be obtained in continuous flow reactors.

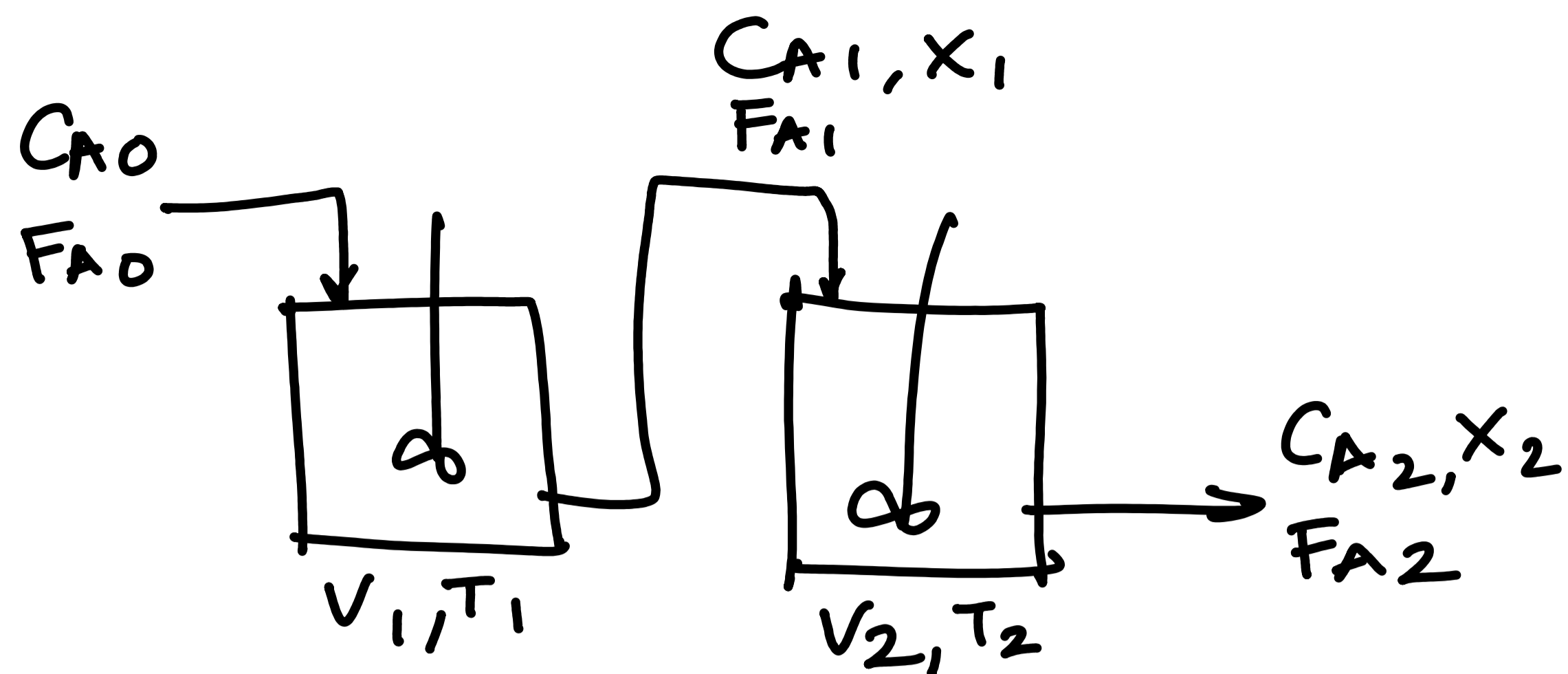
$$Da = \frac{\text{rate of reaction at entry}}{\text{Entering flow rate of A}}$$

$$Da_1 = \tau k ; \quad Da_2 = \tau k C_{A0}$$

If $Da < 1$, then $X < 0.1$

If $Da > 10$, then $X > 0.9$

CSTR in series



First order reaction

$$X = 1 - \frac{1}{(1 + Da_1)^n}$$

For 1st order reaction

$$X_1 = \frac{C_{A1}}{C_{A0}} = \frac{1}{1 + \tau_1 k_1} \Rightarrow C_{A1} = \frac{C_{A0}}{1 + \tau_1 k_1}$$

For 2nd reactor

$$V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}} = \frac{V_0 (C_{A1} - C_{A2})}{k_2 C_{A2}}$$

$$C_{A2} = \frac{C_{A1}}{1 + \tau_2 k_2}$$

$$\Rightarrow C_{A2} = \frac{C_{A0}}{(1 + \tau_2 k_2)(1 + \tau_1 k_1)}$$

If the reactors are equal sized and operate at same T

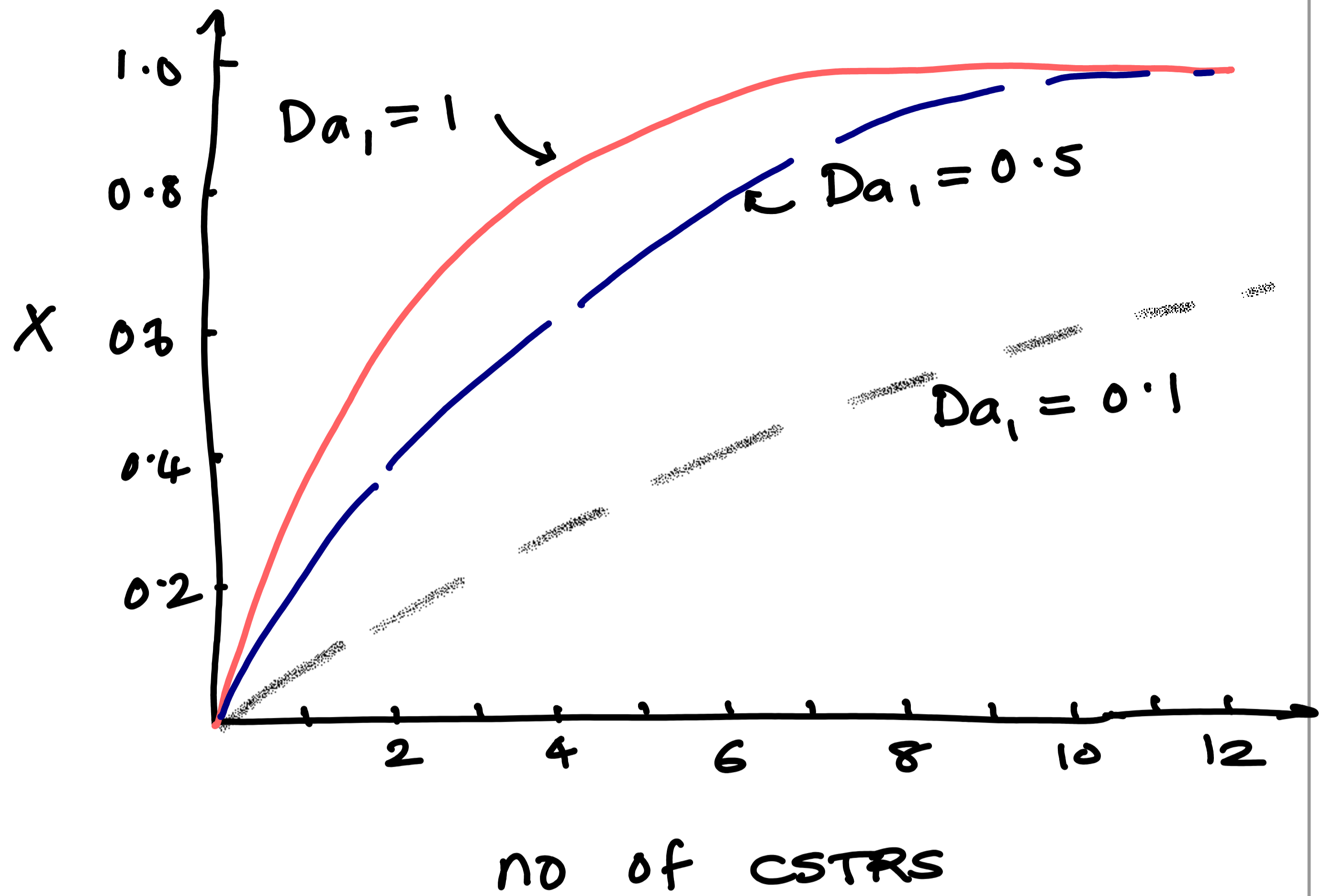
$$C_{A2} = \frac{C_{A0}}{(1 + \tau k)^2} = \frac{C_{A0}}{(1 + Da_1)^2}$$

For n reactors in series

$$X = 1 - \frac{1}{(1 + Da_1)^n}$$

For large Da_1
 \Rightarrow Small no. of reactors are sufficient to achieve high conversion

For small Da_1
 \Rightarrow increasing no. of reactors increases conversion significantly.



Plug flow reactors

Must use the differential form if there is significant pressure drop.

Mole balance

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

$$V = F_{A0} \int_0^X \frac{dX}{-r_A} \quad \dots \left. \vphantom{\int} \right\} \text{No pressure drop}$$

2nd order reaction

$2A \rightarrow \text{products}$

$$-r_A = k C_A^2$$

Liquid phase PFR $v = v_0$

$$\frac{dx}{dv} = \frac{k C_A^2}{F_{A0}}$$

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

$$F_{A0} = C_{A0} v_0$$

$$\therefore v = \frac{v_0}{k C_{A0}} \int_0^x \frac{dx}{(1-x)^2}$$

$$v = \frac{v_0}{k C_{A0}} \left(\frac{x}{1-x} \right)$$

$$X = \frac{\tau k C_{A0}}{1 + \tau k C_{A0}} = \frac{Da_2}{1 + Da_2}$$

gas phase:
→ consider changes in moles, pressure, temperature

Gas phase PFR

$$v = v_0 (1 + \epsilon X) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right)$$

Change in moles

Temp

pressure

For const P & T

$$v = v_0 (1 + \epsilon X)$$

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v_0(1+\epsilon X)}$$

$$C_A = C_{A0} \frac{(1-X)}{(1+\epsilon X)}$$

Combining

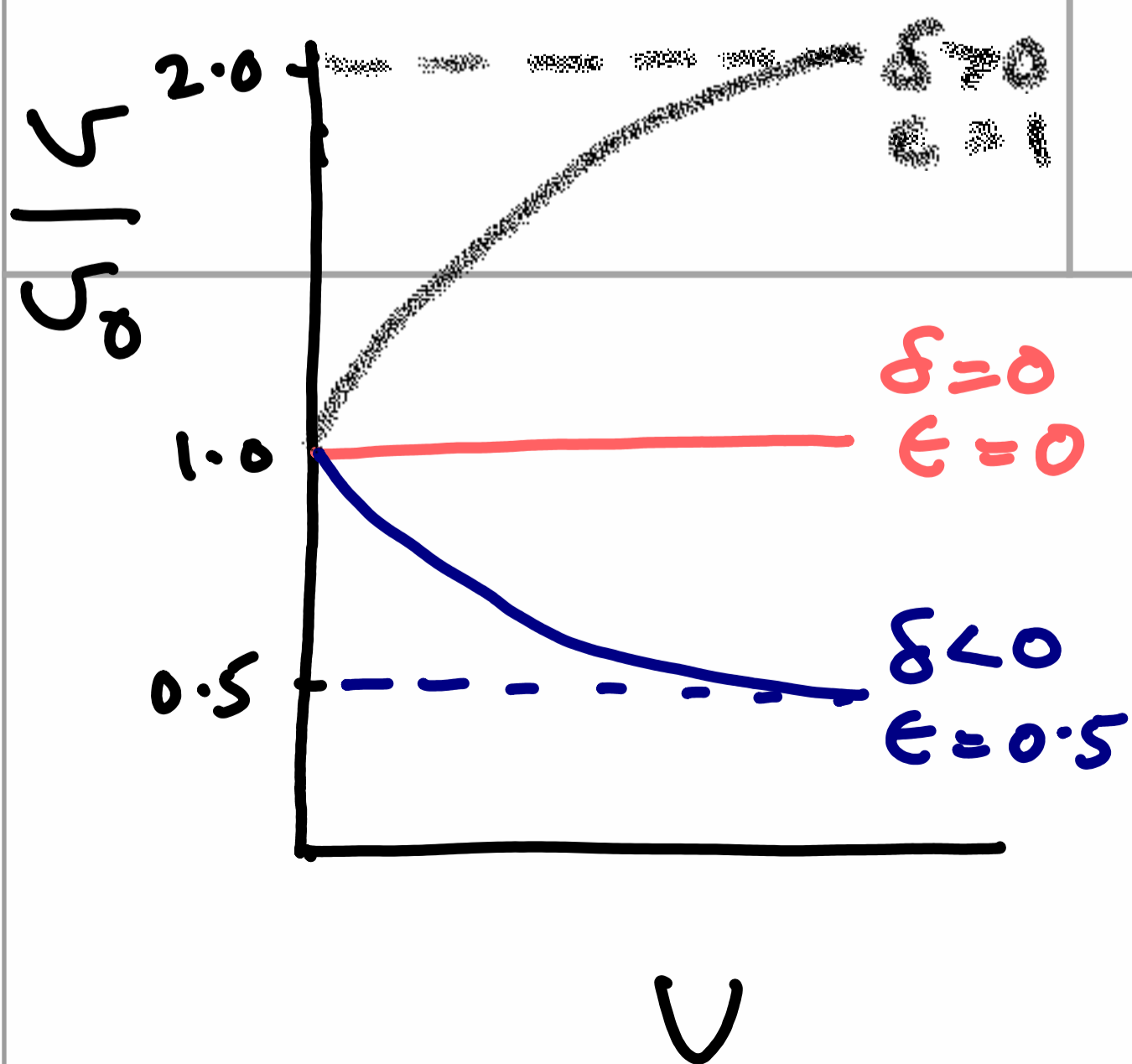
$$V = F_{A0} \int_0^X \frac{(1+\epsilon X)^2}{k C_{A0}^2 (1-X)^2} dX$$

$$V = \frac{v_0}{k C_{A0}} \int_0^X \frac{(1+\epsilon X)^2}{(1-X)^2} dX$$

Evaluate

$$V = \frac{v_0}{k C_{A0}} \left[2\epsilon(1+\epsilon) \ln(1-X) + \epsilon^2 X + \frac{(1+\epsilon)^2 X}{1-X} \right]$$

Effect of ϵ on X



No change in no. of moles = Fluid moves at const. v as X increases

$\epsilon < 0$: decrease in no. of moles

$\Rightarrow v$ decreases as X increases

\Rightarrow longer τ / smaller V for same X

$\epsilon > 0$: increase in no. of moles

$\Rightarrow v$ increases as X increases

\Rightarrow smaller τ / $X < X$ at $v = v_0$

Pressure drop in reactors

Liquid phase
⇒ ignore effect of pressure as Conc. not affected by P

For gas phase reactions
 $C \propto P \Rightarrow$ must account for pressure drop.

Consider reaction in a PBR



Mole balance:

$$F_{A0} \frac{dX}{dW} = -r'_A$$

Rate law:

$$-r'_A = kC_A^2$$

Stoichiometry:

$$C_A = \frac{C_{A0}(1-X)}{(1+\epsilon X)} \left(\frac{P}{P_0} \right) \left(\frac{T_0}{T} \right)$$

combine:

$$\frac{dX}{dW} = \frac{kC_{A0}}{v_0} \left(\frac{1-X}{1+\epsilon X} \right)^2 \left(\frac{P}{P_0} \right)^2$$

$$\Rightarrow \frac{dX}{dW} = f(X, P)$$

Need equation for P

isothermal reactor $T=T_0$

Flow through packed bed

Only gas density varies with pressure

Ergun Equation

$$\frac{dP}{dz} = \frac{-G}{\rho g_c D_p} \left(\frac{1-\phi}{\phi^3} \right) \left[\underbrace{\frac{150(1-\phi)\mu}{D_p}}_{\text{Term 1}} + \underbrace{1.75G}_{\text{Term 2}} \right]$$

P : pressure (kPa)

ϕ : porosity = $\frac{\text{vol. of void}}{\text{bed volume}}$

$g_c = 1$

D_p : particle diameter (m)

μ : viscosity (kg/m-s)

G : superficial mass velocity (kg/m²s)
 $= \rho u$

ρ : density of gas (kg/m³)

u : superficial velocity (m/s)
volumetric flow rate / (c/s area)

Z : length of packed bed (m)

Various forms of Ergun equation:

$\beta_0 \rightarrow$ constant depends on the properties of packed bed

Use for multiple reactions

For single reaction
 $\frac{F_T}{F_{T0}} = 1 + \epsilon X$

Packed bed reactors

\rightarrow Mass flow rate is constant

$$\dot{m}_0 = \dot{m} \Rightarrow P_0 v_0 = P v$$

$$\frac{dP}{dz} = -\beta_0 \left(\frac{P_0}{P}\right) \left(\frac{T}{T_0}\right) \frac{F_T}{F_{T0}}$$

In terms of weight of catalyst

$$\frac{dP}{dW} = -\frac{\alpha}{2} \left(\frac{P_0}{P}\right) \left(\frac{T}{T_0}\right) \left(\frac{F_T}{F_{T0}}\right)$$

$$\frac{dP}{dW} = -\frac{\alpha}{2P} \left(\frac{T}{T_0}\right) \left(\frac{F_T}{F_{T0}}\right)$$

$$\alpha = \frac{2\beta_0}{A_c \rho_c (1-\phi) P_0} \quad \left(\text{unit } \frac{1}{\text{kg}}\right)$$

$$P = P/P_0$$

$$\frac{dP}{dW} = -\frac{\alpha}{2P} \left(\frac{T}{T_0}\right) (1 + \epsilon X)$$

\Rightarrow solve mole balance and the pressure drop equation simultaneously.