When reactants must diffuse inside catalyst pellet in order to react

→ Conc. at the pore mouth must be higher than that inside the pore

→ Entire catalyst surface is not accessible to the same concentration

→ Rate of reaction will vary throughout the pellet.

This chapter

→ Diffusion and rxn in homogeneous systems

→ diffusion and rxn in spherical catalyst pellets

→ Internal effectiveness factor

→ Falsified kinetics

→ Estimation of diffusion- and rxn- limited regimes

→ Mass transfer and rxn in packed bed

→ determination of limiting situations from reaction rate data.

Notes on
Elements of chemical reaction engineering, H. Scott Fogler
- Ranjeet Utikar

Diffusion and reaction in homogeneous systems

— Mole balance on species A for 1D diffusion at steady state

$$-\frac{dW_{Az}}{dz} + r_A = 0$$

$$W_{Az} = -\mathcal{D}_{AB}\frac{dC_A}{dz}$$

$$\mathcal{D}_{AB}\frac{d^2C_A}{dz^2} + r_A = 0$$
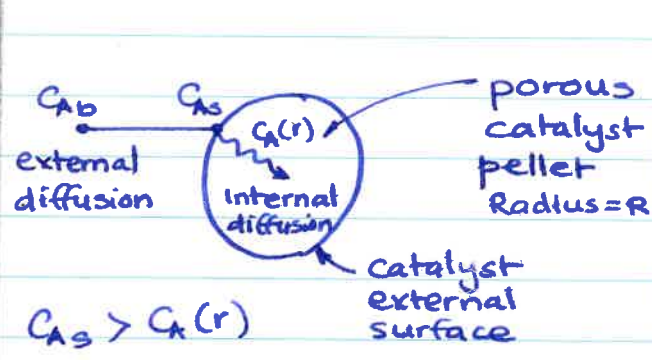
diffusion with chemical reaction
 → Applications
   → medicine
   → cancer treatment using drug laced particulates
   → tissue engineering

# Diffusion and reaction in spherical catalyst pellets

- heterogeneous system

- Reaction seq.
  → external diffusion
  → internal diffusion
  → surface reaction

C_{Ab} C_{As} $C_A(r)$

external diffusion

internal diffusion

porous catalyst pellet
Radius = R

catalyst external surface

$C_{As} > C_A(r)$

consider irreversible isomerization reaction

$$A \longrightarrow B$$
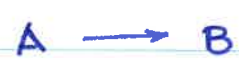
→ reaction occurs on the surface of pore walls within the spherical pellet of radius R

porous catalyst pellet

C_{As}

R r $r+\Delta r$
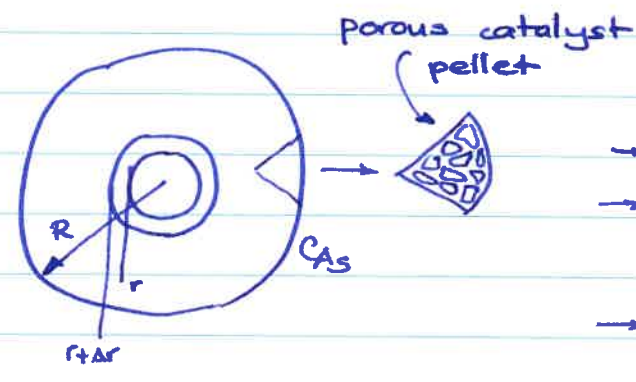
→ Steady state
→ Spherical coordinates
→ constant P & T

Steady state mole balance on a Spherical shell $(r \rightarrow r+\Delta r)$

$$\begin{bmatrix} \text{molar flow} \\ \text{in} \end{bmatrix} - \begin{bmatrix} \text{molar flow} \\ \text{out} \end{bmatrix} + \begin{bmatrix} \text{rate of} \\ \text{reaction} \end{bmatrix} = \begin{bmatrix} \text{rate of} \\ \text{accumulation} \end{bmatrix}$$

area: total area normal to direction of flux

rate of A in at $r = W_{Ar} \cdot 4\pi r^2 \big|_r$

rate of A out at $r+\Delta r = W_{Ar} \, 4\pi r^2 \big|_{r+\Delta r}$

$$\begin{array}{l} \text{rate of generation} \\ \text{of A within a shell} \\ \text{thickness of } \Delta r \end{array} = \begin{bmatrix} \dfrac{\text{reaction rate}}{\text{mass of cat.}} \end{bmatrix} \times \begin{bmatrix} \dfrac{\text{mass of cat}}{\text{vol. of}} \end{bmatrix} \cdot \begin{array}{l} \text{volume} \\ \text{of shell} \end{array}$$

$$= r'_A \cdot \rho_c \cdot 4\pi r_m^2 \, \Delta r$$

r_m: mean radius between r and $r+\Delta r$
used to approximate ΔV

$\therefore \left(W_{Ar} \cdot 4\pi r_1^2\big|_r\right) - \left(W_{Ar} \cdot 4\pi r^2\big|_{r+\Delta r}\right) + r'_A \, \rho_c \, 4\pi r_m^2 \, \Delta r = 0$

dividing by $-4\pi \Delta r$ and taking limit
as $\Delta r \rightarrow 0$

$$\boxed{\dfrac{d\,W_{Ar}\,r^2}{dr} - r'_A\,\rho_c\,r^2 = 0} \quad\text{———} \quad ①$$

EMCD : $\qquad W_{Ar} = -D_e\,\dfrac{dC_A}{dr}$:

Effective diffusivity D_e

→ To reach the inner surface, the reactant A must diffuse from a higher reactant conc. at the pellet external surface into and through the pores of pellet which are at lower concentration.

→ The pores are not straight and cylindrical

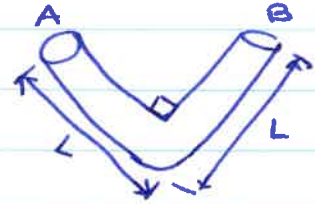→ Effective diffusion coefficient → average diffusion taking place at any interior position in the pellet.

$$D_e = \frac{D_{AB}\,\Phi_P\,\sigma_c}{\tau}$$

τ = tortuosity ; $\quad \sigma_c$: constriction factor
Φ_P = porosity
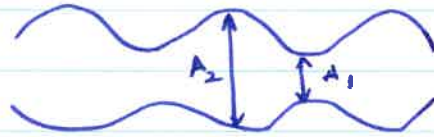
$$\beta = \frac{\text{area } A_2}{\text{area } A_1} \quad ; \sigma_c = f(\beta)$$

constriction

tortuosity

$$\tilde{\tau} = \frac{\text{actual dist. a molecule travels between 2pt}}{\text{shortest distance bet}^n \text{ the two pts.}}$$

$$\Phi_p = \frac{\text{vol. of void space}}{\text{volume of pellet}}$$

$\sigma_c = $ accounts for variation in the

cross-sectional area   at $\beta = 10 \quad \sigma_c = 0.5$

at $\beta = 1 \quad \sigma_c = 1.$

D_e accounts for:

1. Not all the area normal to the direction
   of flux is available for diffusion

2. The paths are tortuous

3. The pores are of varying cross section

Eq. ① can be written as

$$\frac{d\left[-D_e (dC_A/dr) \, r^2\right]}{dr} - r^2 \rho_c \, r_A' = 0 \qquad — ②$$

Rate of reaction

$-r_A$: $mol/dm^3 s$ ... per unit volume

$-r_A'$: $mol/g\text{-}cat\ s$ ... per unit mass of cat.

$-r_A''$: $mol/m^2 s$ ... per unit surface area

S_a : $m^2/g\text{-}cat$ ... $\underline{\text{surface area of catalyst}}$
$\qquad \sim 150\ m^2/g$ $\qquad$ unit mass of catalyst.

$-r_A' = S_a\,(-r_A'')$

$-r_A = \rho_c\,(r_A') = \rho_c S_A\,(-r_A'')$

at high temperatures :

$\quad -r_A'' = k_n''\,C_A^n$

For first order catalytic reaction

k_1 : $1/s$ $\quad \therefore$ $k_1'' S_a \rho_c$: per unit pellet vol.

k_1' : $m^3/kg\ s$: $k_1'' S_a$ $\qquad$: per unit mass

k_1'' : m/s $\qquad\qquad$: per unit surface area

Substituting the rate law in ②

$$\frac{d\left[r^2(-\mathcal{D}_e\,dC_A/dr)\right]}{dr} + r^2\,\overbrace{k_n'' S_a \rho_c}^{k_n}\,C_A^n = 0$$

dividing by $-r^2 \mathcal{D}_e$

$$\frac{d^2 C_A}{dr^2} + \frac{2}{r}\left(\frac{dC_A}{dr}\right) - \frac{k_n}{D_e} C_A^n = 0 \quad\text{——} \quad ③$$

Boundary conditions

1. Conc. is finite at the centre

   C_A is finite at $r = 0$

2. $C_A = C_{AS}$ at $r = R$

Dimensionless form of reaction-diffusion equation

Let $\psi = \dfrac{C_A}{C_{AS}}$ and $\lambda = \dfrac{r}{R}$

BCs: at $\lambda = 0$ ψ is finite

at $\lambda = 1$ $\psi = 1$

$$W_{Ar} = -D_e \frac{dC_A}{dr}$$

$$\frac{dC_A}{dr} = \frac{dC_A}{d\lambda} \cdot \frac{d\lambda}{dr} = \frac{d\psi}{dC_A} \frac{dC_A}{d\psi} \frac{d\lambda}{dr}$$

$$\frac{dC_A}{d\psi} = C_{AS} \quad ; \quad \frac{d\lambda}{dr} = \frac{1}{R}$$

$$\therefore \quad \frac{dC_A}{dr} = \frac{d\psi}{d\lambda} \frac{C_{As}}{R} \qquad —④$$

and

$$W_{Ar} = -D_e \frac{dC_A}{dr} = -\frac{D_e C_{As}}{R}\left(\frac{d\psi}{d\lambda}\right)$$

differentiating ④

$$\frac{d^2 C_A}{dr^2} = \frac{d}{dr}\left(\frac{dC_A}{dr}\right) = \frac{d}{d\lambda}\left(\frac{d\psi}{d\lambda}\frac{C_{As}}{R}\right)\frac{d\lambda}{dr}$$

$$\frac{d^2 C_A}{dr^2} = \frac{d^2\psi}{d\lambda^2}\left(\frac{C_{As}}{R^2}\right) \qquad —⑤$$

$\therefore$ Eq. ③ in dimensionless form

$$\frac{d^2\psi}{d\lambda^2} + \frac{2}{\lambda}\frac{d\psi}{d\lambda} - \frac{k_n R^2 C_{As}^{n-1}}{D_e}\psi^n = 0$$

$$\boxed{\frac{d^2\psi}{d\lambda^2} + \frac{2}{\lambda}\frac{d\psi}{d\lambda} - \phi_n^2 \psi^n = 0} \quad —⑥$$

$$\boxed{\phi_n^2 = \frac{k_n R^2 C_{As}^{n-1}}{D_e}} \quad \dots \text{Thiele} : \phi_n \text{ modulus}$$

$$= \frac{\text{'a' surface reaction rate}}{\text{'a' diffusion rate}}$$

When Thiele modulus is large
→ Internal diffusion limits overall reaction

When Thiele modulus is small
→ Surface reaction is rate limiting.

For first order reaction equation ⑥ becomes

$$\frac{d^2\psi}{d\lambda^2} + \frac{2}{\lambda}\frac{d\psi}{d\lambda} - \phi_1^2\psi = 0 \qquad - ⑦$$

$$\phi_1 = R\sqrt{\frac{k_1}{D_e}} \qquad - ⑧$$

BCs : $\psi = 1$ at $\lambda = 1$

ψ is finite at $\lambda = 0$

Let $y = \psi\lambda$

$\therefore \quad \frac{d\psi}{d\lambda} = \frac{1}{\lambda}\left(\frac{dy}{d\lambda}\right) - \frac{y}{\lambda^2}$

$\frac{d^2\psi}{d\lambda^2} = \frac{1}{\lambda}\left(\frac{d^2y}{d\lambda^2}\right) - \frac{2}{\lambda^2}\left(\frac{dy}{d\lambda}\right) + \frac{2y}{\lambda^3}$

with these transformations eq. ⑦ becomes

$$\frac{d^2y}{d\lambda^2} - \Phi_1^2 y = 0$$

This differential equation has following solution

$$y = A_1 \cosh \Phi_1 \lambda + B_1 \sinh \Phi_1 \lambda$$
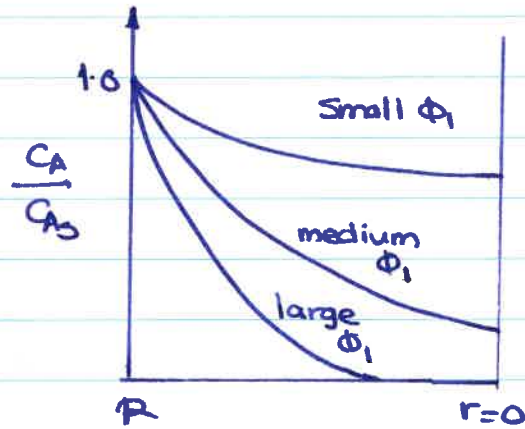
In terms of Ψ

$$\Psi = \frac{A_1}{\lambda} \cosh \Phi_1 \lambda + \frac{B_1}{\lambda} \sinh \Phi_1 \lambda$$

at $\lambda = 0$

$$\cosh \Phi_1 \lambda \longrightarrow 1$$
$$\sinh \Phi_1 \lambda \longrightarrow 0$$
$$1/\lambda \longrightarrow \infty$$

at $\lambda = 0$ Ψ is finite $\therefore$ A_1 must be zero

at $\lambda = 1$ $\Psi = 1$ $\therefore$ $B_1 = \frac{1}{\sinh \Phi_1}$

$\therefore$

$$\boxed{\Psi = \frac{C_A}{C_{As}} = \frac{1}{\lambda} \frac{\sinh \Phi_1 \lambda}{\sinh \Phi_1}} \qquad \longrightarrow ⑨$$

Small ϕ_1: surface rxn controls.
- Significant amount of reactant diffuses well into pellet interior
- Conc. profile is shallow
- virtually entire internal surface is accessible to C_{AS}

Large ϕ_i : reaction is rapid
- reactant is consumed very close to the catalyst external surface
- very little penetrates into the pellet
- If a porous pellet is to be plated with a precious metal catalyst (e.g. Pt) it should only be plated in the immediate vicinity of external surface.

Internal effectiveness factor (η)

η is a measure of how far the reactant diffuses into the pellet before reacting.

$$\eta = \frac{\text{actual overall rate of reaction}}{\text{rate of reaction if entire interior surface was at } C_{AS}}$$

$$\eta = \frac{-r_A}{-r_{AS}} = \frac{-r'_A}{-r'_{AS}} = \frac{-r''_A}{-r''_{AS}}$$

Effectiveness factor for 1st order reaction

$$\eta = \frac{-r_A}{-r_{AS}} = \frac{-r_A \cdot \text{vol of particle}}{-r'_A \cdot \text{vol. of particle}} = \frac{M_A}{M_{AS}}$$

$$M_{AS} = \frac{\text{rate at external surface}}{\text{volume}} \times \frac{\text{vol. of}}{\text{catalyst pellet}}$$

$$= -r_{AS}\left(\frac{4}{3}\pi R^3\right) = k_1 C_{AS}\left(\frac{4}{3}\pi R^3\right)$$

at external surface $\lambda = 1$

Actual rate of reaction

$$M_A = 4\pi R D_e C_{AS} \left.\frac{d\psi}{d\lambda}\right|_{\lambda=1}$$

At steady state

Net flow of $=$ reaction
species A that within
enters into the the pellet
pellet at the
external pellet
surface

$\therefore$ overall rate $=$ total molar flow into
of reaction the catalyst pellet

$$M_A = -4\pi R^2 \, W_{Ar}\Big|_{r=R}$$

$$= +4\pi R^2 \, \frac{dC_A}{dr}\Big|_{r=R}$$

$$M_A = 4\pi R \, \vartheta_e \, C_{AS} \, \frac{d\psi}{d\lambda}\Big|_{\lambda=1}$$

Differentiating ⑨

$$\frac{d\psi}{d\lambda}\Big|_{\lambda=1} = \left(\frac{\phi_1 \cosh \lambda\phi_1}{\lambda \sinh \phi_1} - \frac{1}{\lambda^2} \frac{\sinh \lambda \phi_1}{\sinh \phi_1}\right)_{\lambda=1}$$

$$= \phi_1 \coth \phi_1 - 1$$

$$\eta = \frac{M_A}{M_{AS}} = \frac{4\pi R \mathcal{D}_e C_{AS}}{k_1 C_{AS} \frac{4}{3}\pi R^3}(\phi_1 \coth \phi_1 - 1)$$
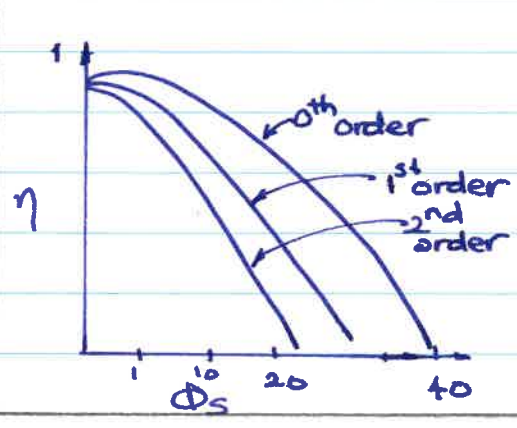
$$= \frac{3}{(k_1 R^2 / \mathcal{D}_e)}(\phi_1 \coth \phi_1 - 1)$$

$$\therefore \quad \boxed{\eta = \frac{3}{\phi_1^2}(\phi_1 \coth \phi_1 - 1)}$$

$$\phi_1 = R\sqrt{\frac{k_1}{\mathcal{D}_e}}$$

If $\quad \phi_1 > 2 \qquad \eta \simeq \frac{3}{\phi_1^2}[\phi_1 - 1]$

If $\quad \phi_1 > 20 \qquad \eta \simeq \frac{3}{\phi_1}$

0th order $\phi_{SO} = R\sqrt{\dfrac{k_0}{\mathcal{D}_e C_{AO}}}$

$\phi_{S1} = R\sqrt{k_1/\mathcal{D}_e}$

$\phi_{S2} = R\sqrt{k_2 C_{AO}/\mathcal{D}_e}$

η vs ϕ plot with "reaction rate limited" and "Internal diffusion limited" regions.
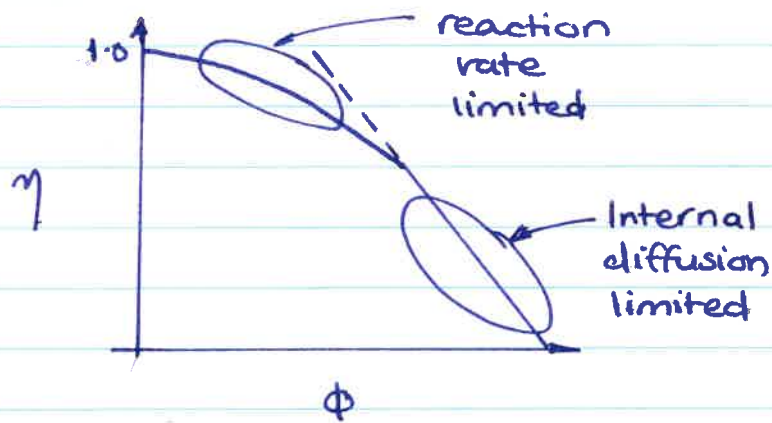
Weisz-Prater criteria for internal diffusion limitation

$$C_{WP} = \eta \phi_1^2 = 3 (\phi \coth \phi_1 - 1)$$

$$= \frac{\text{actual reaction rate}}{\text{rate evaluated at } C_{As}} \cdot \frac{\text{rate at } C_{As}}{A \text{ diffusion rate}}$$
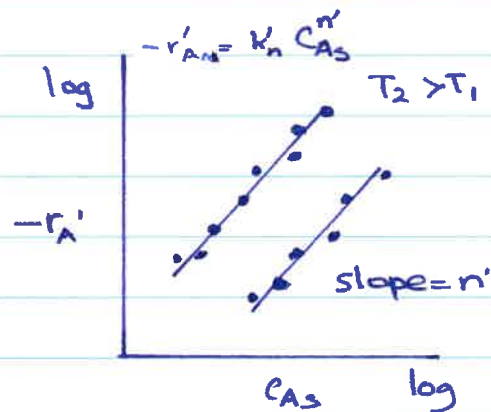
$$C_{WP} = \frac{\text{actual reaction rate}}{A \text{ diffusion rate.}}$$

$C_{WP} \ll 1$: No diffusion limitations

$C_{WP} \gg 1$: Severe diffusion limitation

Falsified kinetics

→ Measured reaction order and activation energy are not the true values.

$$-r'_{A_n} = k_n C^n_{AS}$$

$T_2 > T_1$

slope = n'

$\log -r_A'$ vs C_{AS} $\log$

→ reaction rate data at two different temp. T_1 & T_2

→ differential reactor

→ no external mass transfer resistance

→ observed order n'

→ Relation between the true reaction order n and measured order n'

Actual rate
$$-r_A' = \eta(-r'_{AS})$$
$$= \eta(k_n C^n_{AS})$$

For large values of thiele modulus ϕ_n → internal mass transfer is limiting $\eta = 3/\phi_n$
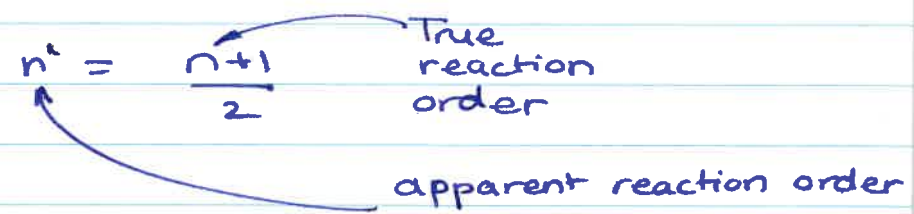
$$-r_A' = \frac{3}{\phi_n}\sqrt{\frac{2}{n+1}}\, k_n C^n_{AS}$$

$$-r_A' = \frac{3}{R}\sqrt{\frac{\mathcal{D}e}{k_n}\, C_{AS}^{1-n}}\;\sqrt{\frac{2}{n+1}\, k_n C_{AS}^{n}}$$

$$\therefore \quad -r_A' = \frac{3}{R}\sqrt{\frac{2\mathcal{D}e}{(n+1)}}\; k_n^{1/2}\, C_{AS}^{(n+1)/2}$$

$$-r_A' = \sqrt{\frac{2}{n+1}}\underbrace{\left(\frac{3}{R}\sqrt{\mathcal{D}e}\; k_n^{1/2}\, C_{AS}^{(n+1)/2}\right)}_{actual} = \underbrace{k_n'\, C_{AS}^{n'}}_{measured}$$

$$\therefore \quad C_{AS}^{\frac{n+1}{2}} = C_{AS}^{n'} \quad\Rightarrow\quad \boxed{n_{True} = 2\, n_{app} - 1}$$

$$n' = \frac{n+1}{2} \quad\leftarrow\; \text{True reaction order}$$

apparent reaction order

$$k_n' = A_{App}\, e^{-E_{app}/RT} \qquad\qquad k_n = A_T\, e^{-E_T/RT}$$

$$-r_A = \left(\frac{3}{R}\sqrt{\frac{2\mathcal{D}e}{n+1}}\right) A_T^{1/2}\left[\exp\left(\frac{-E_T}{RT}\right)\right]^{1/2} C_{AS}^{(n+1)/2} = A_{app}\, e^{-E_{app}/RT}\, C_{AS}^{n'}$$

taking log

$$\ln\left[\frac{3}{R}\sqrt{\frac{2 \mathcal{D}e}{n+1}}\ A_T^{1/2}\ C_{AS}^{(n+1)/2}\right] - \frac{E_T}{2RT} = \ln\left[A_{app}\ C_{AS}^{n'}\right] - \frac{E_{app}}{RT}$$

$$\Rightarrow \qquad \frac{E_{app}}{RT} = \frac{E_T}{2RT}$$

$$\boxed{E_T = 2\,E_{APP}}$$

$\Rightarrow$ The measurement of the apparent reaction order and activation energy results in presence of internal diffusion limitations and is referred to as falsified or disguised kinetics.

Higher activation energy

$\Rightarrow$ Reaction becomes more sensitive to temperature

$\Rightarrow$ Possibility of runaway conditions

$\Rightarrow$ explosion

Overall effectiveness factor (Ω)

→ Both internal and external mass transfer limitations are considered.
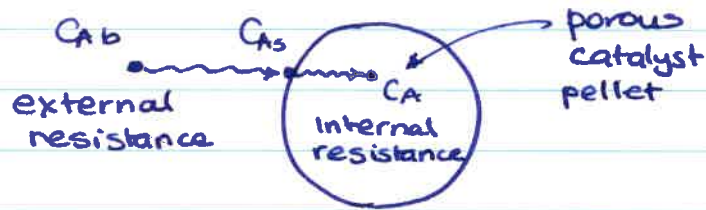
Molar rate of mass transfer from bulk fluid to the external surface

$$= \begin{bmatrix} \text{molar} \\ \text{flux} \end{bmatrix} \times \begin{bmatrix} \text{surface} \\ \text{area} \end{bmatrix}$$

$$M_A = W_{Ar} \cdot a_c \Delta V$$

= net rate of reaction on and within the pellet

$$= -r_A'' \, (\text{external area} + \text{internal area})$$

External area $= a_c \Delta V$

Internal area $\doteq S_a \underbrace{\rho_c (1-\phi) \Delta V}_{\rho_b}$

$$= S_a \rho_b \Delta V$$

$$\therefore \quad M_A = -r_A'' \left[\quad a_c \Delta V + S_a \rho_b \Delta V \right]$$

$$\therefore \quad W_{Ar}\, a_c = -r_A''\,(a_c + S_a \rho_b)$$

For most catalyst $\quad a_c \ll S_a \rho_b$

$$\therefore \quad W_{Ar}\, a_c = -r_A''\, S_a \rho_b$$

$$-r_A' = -r_A''\, S_a$$
$$-r_A = -r_A''\, \rho_b$$

$$\therefore \quad W_{Az}\, a_c = -r_A = -r_A''\, S_a \rho_b$$

Rate of mass transport to external surface

$$M_A = W_{Ar}\, a_c \Delta V = k_c (C_{Ab} - C_{As})\, a_c \Delta V$$

$$-r_A = \eta\, r_{As}$$
$$= \eta\, k_1 C_{As} \qquad k_1 = k_1''\, S_a \rho_b$$

Need to eliminate C_{As}

$$\therefore \quad k_c (C_{Ab} - C_{As})\, a_c = \eta\, k_1 C_{As}$$

$$\rightarrow \quad -r_A = \frac{\eta\, k_1 k_c\, a_c\, C_{Ab}}{k_c a_c + \eta k_1}$$

$$\boxed{\eta = \frac{\text{actual reaction rate}}{\text{rate at } C_{AS}, T_S}}$$

$$\Omega = \frac{\text{actual reaction rate}}{\text{rate at } C_{Ab}, T_b}$$

$$-r_A = \frac{\eta}{1 + \frac{\eta k_1}{k_c a_c}} k_1 C_{Ab}$$

$$= \Omega k_1 C_{Ab}$$

$$\boxed{\Omega = \frac{\eta}{1 + \frac{\eta k_1}{k_c a_c}}}$$

For high flowrate of fluid
k_c is large $\Rightarrow 1 \gg \dfrac{\eta k_1}{k_c a_c}$

$$\Omega = \eta$$

Determination of limiting situations from reaction rate data

type of limitation	variation of reaction rate with		
	velocity	particle size	temperature
External diffusion	$U^{1/2}$	$d_p^{-3/2}$	$\approx$ linear
Internal diffusion	Independent	d_p^{-1}	exponential
Surface reaction	independent	Independent	exponential

External mass transfer

$$k_c \propto \frac{U^{1/2}}{d_p^{1/2}} \qquad\qquad -r'_A = k_c a_c C_A$$

$$a \propto \frac{1}{d_p} \qquad\qquad \left(a_c = \frac{6(1-\Phi)}{d_p} \right)$$

$$\therefore \quad -r'_A \propto \frac{U^{1/2}}{d_p^{3/2}}$$

For gas phase reaction in packed bed
$$k_c \propto U^{1/2} T^{11/12} \quad\Rightarrow\quad -r'_A \propto T$$

Internal diffusion

$$-r_A' = \frac{3}{R} \sqrt{\frac{2 D_e}{(n+1)}} \; k_n^{1/2} \; c_{As}^{(n+1)/2}$$

$$-r_A' \propto \frac{1}{d_p}$$

- $-r_A'$ exhibits an exponential temperature dependence
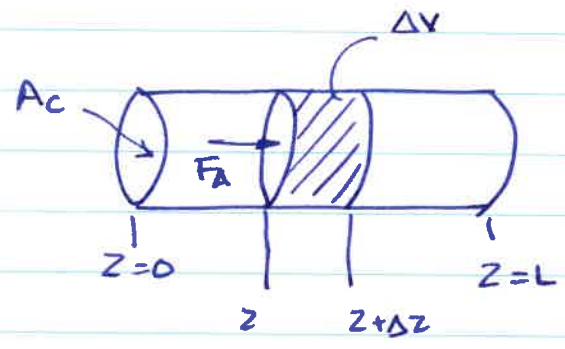 → Not as strong as that for surface reaction

Activation energy

→ $8 - 24 \; kJ/mol$ ⇒ most likely strongly diffusion limited

→ $> 200 \; kJ/mol$ ⇒ reaction rate limited.

Mass transfer and reaction in packed bed

shell balance at steady state

$$\begin{bmatrix} \text{rate} \\ \text{in} \end{bmatrix} - \begin{bmatrix} \text{rate} \\ \text{out} \end{bmatrix} + \begin{bmatrix} \text{rate of} \\ \text{formation of A} \end{bmatrix} = 0$$

$$A_c W_{Az}\big|_z - A_c W_{Az}\big|_{z+\Delta z} + r_A' \rho_b A_c \Delta z = 0$$

dividing by $A_c \Delta z$ and taking limit as $\Delta z \rightarrow 0$

$$-\frac{dW_{Az}}{dz} + \overbrace{r_A' \rho_b}^{r_A} = 0 \qquad \text{——} \textcircled{1}$$

$$W_{Az} = -\mathcal{D}_{AB} \frac{dC_{Ab}}{dz} + y_{Ab}(W_{Az} + W_{Bz})$$

$$\qquad\qquad\qquad J_A \quad + \quad B_A$$

$$B_{Az} = y_{Ab}(W_{Az} + W_{Bz}) = y_{Ab} c U$$

$$= U C_{Ab}$$

∴ equation ① becomes

$$D_{AB} \frac{d^2 C_A}{dz^2} - U \frac{d C_A}{dz} + r_A = 0 \qquad —②$$

⌣ diffusion / dispersion in axial
direction

$$D_{AB} \to D_a$$

$$-r_A = \Omega(r_{Ab})$$

For 1st order kinetics

$$-r_A = \Omega k_1 C_{Ab}$$

∴ ② becomes

$$\boxed{D_a \frac{d^2 C_{Ab}}{dz^2} - U \frac{d C_{Ab}}{dz} - \Omega k_1 C_{Ab} = 0} \qquad —③$$

Neglecting axial dispersion

$$\left| U \frac{dC_{Ab}}{dz} \right| \gg \left| D_{a} \frac{d^2 C_{Ab}}{dz^2} \right|$$

$$\frac{dC_{Ab}}{dz} = \frac{-\Omega k_1 C_{Ab}}{U}$$

$$C_{Ab} = C_{Ab0} \quad \text{at} \quad z = 0$$

$$\Rightarrow \quad C_{Ab} = C_{Ab0} \exp\left[\frac{-\Omega k_1 z}{U}\right]$$

$$\boxed{X = 1 - \frac{C_{Ab}}{C_{Ab0}} = 1 - \exp\left[\frac{-k_1 \Omega L}{U}\right]}$$