Effect of Temperature:

$$-r_A = \frac{k P_A}{1 + K_A P_A + K_B P_B}$$

at high T, $K_A \approx K_B \approx 0$

$-r_A \approx k P_A$ (Pseudo homogenous).

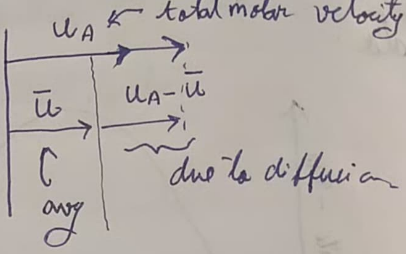
Mass transfer effects on the heterogenous reaction:

$$W_A = W_{Ax}\hat{i} + W_{Ay}\hat{j} + W_{Az}\hat{k}$$

molar flux.

$$W_A = J_A + B_A$$

diffusional Bulk.



$$u_A = \bar{u} + (u_A - \bar{u})$$

So $C_A u_A = C_A \bar{u} + C_A (u_A - \bar{u})$

$$W_A = C_A \left(\frac{u_A C_A + u_B C_B}{C} \right) + C_A (u_A - \bar{u})$$

$\therefore \quad W_A = (W_A + W_B) y_A + J_A$

So. Fick's 1st law:

$$J_A = -D_{AB} (C \nabla y_A)$$

$$\therefore \quad W_A = (W_A + W_B) y_A - D_{AB} C \nabla y_A$$

for equimolar counter diffusion,

$$W_A = -W_B$$

$$W_A = -D_{AB}\, C\, \nabla y_A$$

→ for porous catalyst:

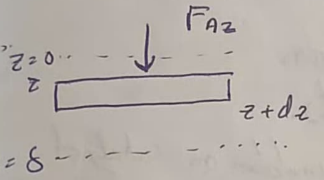
Knudsen diffusion is considered and $W_A = J_A = -D_k \nabla C_A$.

→ Diffusion through stagnant film

$W_B = 0$ [B is stagnant]

$\therefore$ $W_A = J_A + y_A W_A$ as. $W_B = 0$

now,



$z=0,\ C_A = C_{Ab}$

$z=\delta,\ C_A = C_{AS}$

now,

$$\frac{F_{Az} - F_{Az+dz}}{dz} = 0$$

$$\therefore \frac{dF_A}{dz} = 0$$

A_c = area of differential volume dz.

$$F_{Az} = W_{Az} A_c.$$

So

$$\frac{dW_{Az}}{dz} = 0$$

$$\therefore N_A = -D_{AB}\frac{dC_A}{dz}$$

$$\therefore \frac{dW_A}{dz} = -D_{AB}\frac{d^2C_A}{dz^2}$$

P.T.O.

for Heat transfer

$$Nu = 2 + 0.6\, Re^{1/2} Pr^{1/3}$$

Similarly for mass transfer

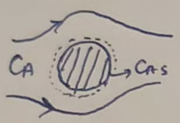
$$Sh = 2 + 0.6\, Re^{0.5} Pr^{1/3}$$

$$\therefore W_A = k_c (C_{Ab} - C_{As})$$

$$Sh = \frac{k_c d_p}{D_{AB}} \quad , \quad Nu = \frac{h d_p}{k_t}$$

$$Pr = \frac{\upsilon}{D_{AB}}$$

visualize:



In Boundary layer,
MT resistance exits.
at eqm no accumulation on catalyst.
(on the surface)

Boundary conditions:

On the surface: $N_A = -r'_A$

at the Boundary layer $= k_c (C_A - C_{Ao})$

$$W_A = -r_A = k_c (C_A - C_{As}) = k_r C_{As}$$

$$C_{As} = \frac{k_c C_A}{k_c + k_r}$$

$$-r'_{As} = \frac{k_r k_c C_A}{k_c + k_r}$$

$$\boxed{k_{eff} = \frac{k_r k_c}{k_c + k_r}}$$

If the reaction is Rapid:

MT step is rate limiting

$$-r'_{AS} = \frac{k_c C_A}{1 + \left(\frac{k_c}{k_S}\right)}$$

$$\frac{k_c}{k_S} << 1$$

$$\therefore \quad -r'_{AS} = k_c C_A.$$

$$; \quad Sh \simeq 0.6\, Re^{0.5}\, Sc^{1/3}$$

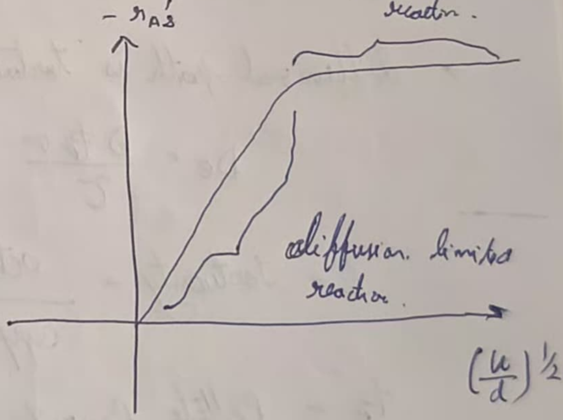
i.e. $$\frac{k_c d_P}{D_{AB}} = 0.6 \left(\frac{d_P U}{\nu}\right)^{1/2} \left(\frac{\nu}{D_{AB}}\right)^{1/3}$$

$$\therefore \quad k_c = 0.6 \frac{(D_{AB})^{2/3}}{\nu^{1/6}} \left(\frac{U}{d_P}\right)^{1/2}$$

for slow reaction:

$$k_S << k_c.$$

$$\therefore \quad -r'_{AS} = k_S C_A.$$



If u is small

→ MT is dominating due to thicker B L.

Mass transfer with reaction in a porous catalyst (Internal diff. Resistance to M. T)

$$D_{AB} = \frac{1}{3} \bar{V} \lambda$$

$$D_K = \frac{2}{3} a \bar{V}.$$

working formula.

$$D_{KA} = 9700\, r \left(\frac{T}{M_A}\right)^{1/2}$$

r in cm.

So.

$$D = \frac{1}{\frac{1}{D_{AB}} + \frac{1}{D_K}}$$

→ If the pore structure inside the catalyst is complicated, then we talk about effective diffusivity.

→ We only consider radial variation of conc. (inside catalyst particle)

→ Radial flux is considered normal to the surface (inside the catalyst pelette)

→ Effective diffusivity considers that not all area normal to ~~of~~ direction of flux are available for molecule to diffuse.

→ Diffusional path is tortuous in nature

$$D_e = \frac{D\, \phi_P\, \sigma}{\tau}$$

τ = Tortuosity = $\frac{\text{actual distance}}{\text{apparent distance}}$.

ϕ_P – Pellete Porosity.

$$f(\beta) = \frac{\text{area } a_2}{\text{area } a_1}$$

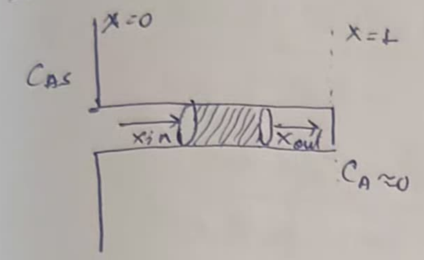
σ = constriction factor.

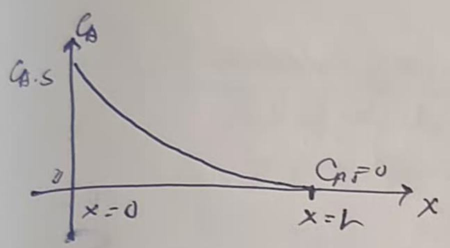
D = Combined diffusivity.

Single cylindrical Pore, Ist order Reaction

now

Flat plate Geometry:





→ At any Position within the pore, the concentration of A is C_A and on the surface it is C_S.

→ At the end of the pore $C_A \simeq 0$. hence no reaction.

where $x=0$, $C_A = C_{AS}$

$x=L$, $\frac{dC_A}{dx} = 0$.

from mole balance.

$$\frac{\left(\frac{dC_A}{dx}\right)_{out} - \left(\frac{dC_A}{dx}\right)_{in}}{\Delta x} = \frac{2 k_s C_A}{rD}$$

$$\therefore \frac{d^2 C_A}{dx^2} - \frac{2 k_s}{rD} C_A = 0$$

$\therefore k_s \cdot S = kV$. & $k = \frac{2 k_s}{r}$

So $\frac{d^2 C_A}{dx^2} - \frac{k C_A}{D} = 0.$

So

$$C_A = m_1 e^{mx} + m_2 e^{-mx}$$

$$m = \sqrt{\frac{k}{D}}.$$

B.C.

$x=0, \quad C_A = C_{AS}$

$x=L, \quad \left.\frac{dC_A}{dx}\right|_{x=L} = 0$

So $\frac{dC_A}{dx} = 0$

$m_1 e^{mx} = m_2 e^{-mx}$

$m_1 e^{2mL} = m_2$

and at $x=0$, $C_A = C_{AS}$

So.

$m_2 = C_{AS} - m_1$

$m_1 e^{2mL} + m_1 = C_{AS}$

$m_1 = \frac{C_{AS}}{1+e^{2mL}} \quad \therefore m_2 = \frac{C_{AS}\, e^{2mL}}{1+e^{2mL}}$

So.

$m_1 = \frac{C_{AS}\, e^{-mL}}{e^{mL}+e^{-mL}}, \quad m_2 = \frac{C_{AS}\, e^{mL}}{e^{mL}+e^{-mL}}$

So.

$$C_A = \frac{C_{AS}}{e^{mL}+e^{-mL}} \left[e^{m(x-L)} + e^{-m(x-L)} \right]$$

$$\Rightarrow C_A = C_{AS} \frac{\cosh[m(L-x)]}{\cosh(mL)}$$

$$\therefore \boxed{\frac{C_A}{C_{AS}} = \frac{\cosh\left[\sqrt{\frac{k}{D}}\,(L-x)\right]}{\cosh\left(\sqrt{\frac{k}{D}}\,L\right)}}$$

Thiele modulus = $mL = \left(\sqrt{\frac{k}{D}}\right)L$

* Effectiveness factor:

$$\eta = \frac{\text{Rate of Reaction with diffusion}}{\text{Rate of Reaction without diffusion}}$$

$$= \frac{\text{rate of reaction within the pore}}{\text{rate of reaction on the catalyst surface}}$$

$$= \frac{\text{observed rate}}{\text{rate of not slowed by pore diffusion}}$$

$$= \frac{r_A}{r_{AS}}.$$

→ If Thiele modulus is small, i.e, $mL < 0.5$, $\eta \approx 1$. (very low Pore resistance, ~~D~small~~ $\underbrace{D \sim \text{high},\ k \sim \text{less},\ L \sim \text{small}}_{\text{3 Possible scenario.}}$)

→ If Thiele modulus is more, i.e, $mL > 5$, $\eta \approx \frac{1}{mL}$ (strong Pore resistance, $\underbrace{D \sim \text{low},\ k \sim \text{more},\ L \sim \text{long}}_{\text{3 Possible scenario.}}$)

1st order reaction,

$$-r_A = k C_A = k \eta C_{AS} \qquad \left[\because \eta = \frac{C_A}{C_{AS}}\right]$$

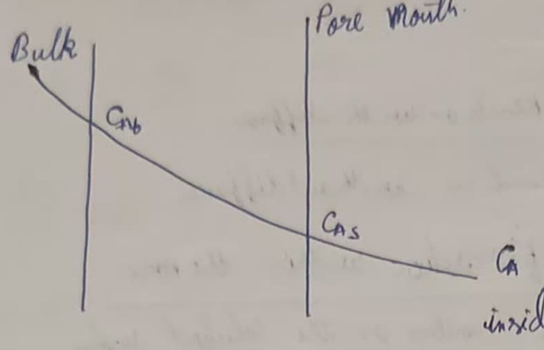
(a) for no resistance of the Pore,

$$-r_A = k C_{AS}.$$

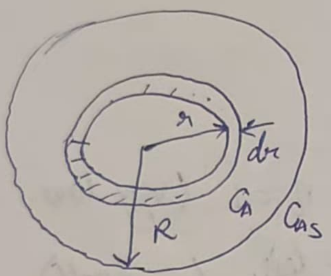
(b) for strong Pore resistance, $-r_A = k\sqrt{\frac{D}{k}}\frac{1}{L} C_{AS}$

$$-r_A = \frac{\sqrt{kD}}{L} C_{AS}$$

Drop in Concentration.



Pore diffusion in a spherical pellet : Effectiveness factor:



pellete having uniform property throughout. isothermal.

mole balance.

output - input + disappearance = $\overset{0}{\text{accumulation}}$.

$$\Rightarrow -4\pi r^2 D_e \left(\frac{dC_A}{dr}\right)\Big|_r - \left(-4\pi r^2 \frac{dC_A}{dr}\right) D_e \Big|_{r+dr} = 4\pi r^2\, dr\, \rho_p k C_A .$$

$$\Rightarrow \frac{d}{dr}\left[4\pi r^2 \frac{dC_A}{dr}\right] = \frac{4\pi r^2 \rho_p k C_A}{D_e}$$

$$\Rightarrow \frac{d}{dr}\left[r^2 \frac{dC_A}{dr}\right] = \frac{r^2 \rho_p k_1 C_A}{D_e}.$$

$k_1 C_A$ = rate of the reaction per unit wt. of the catalyst kmol / kg-cat.s

D_e = effective diffusivity

ρ_p = Catalyst Particle density.

$$\frac{d^2C_A}{dr^2} + \frac{2}{r}\frac{dC_A}{dr} - \frac{\rho_p k_1}{D_e} C_A = 0$$

$$r=0, \quad \frac{dC_A}{dr} = 0$$

$$r=R, \quad C_A = C_{AS}$$

$$, \mathcal{L}\{C_A\} = C.$$

now. $$\mathcal{L}\left\{\frac{d^2C_A}{dx^2}\right\} = s^2 C - s\, C_A(0)$$

$$\mathcal{L}\left\{\frac{1}{r}\frac{dC_A}{dr}\right\} = \int_s^\infty \mathcal{L}\left\{\frac{dC_A}{dr}\right\} d\tilde{s}$$

$$= \int_s^\infty [\tilde{s} C - C_A(0)]\, d\tilde{s}$$

$$\mathcal{L}\left\{-\frac{\rho_p k_1}{D_e} C_A\right\} = -\frac{\rho_p k_1}{D_e} C.$$

So.

$$\Rightarrow s^2 C - s\, C_A(0) + 2\int_s^\infty [\tilde{s} C - C_A(0)]\, d\tilde{s} - \frac{\rho_p k_1}{D_e} C = 0$$

now differentiating.

$$\Rightarrow 2sC + s^2 \frac{dC}{ds} - C_A(0) + 2C_A(0) - 2sC - \frac{\rho_p k_1}{D_e}\frac{dC}{ds} = 0.$$

$$\Rightarrow \left[s^2 - \frac{\rho_p k_1}{D_e}\right]\frac{dC}{ds} = -C_A(0)$$

$$\Rightarrow \frac{dC}{ds} = \frac{-C_A(0)}{s^2 - \frac{\rho_p k_1}{D_e}} = \frac{-C_A(0)}{2\sqrt{\frac{\rho_p k_1}{D_e}}}\left[\frac{1}{s+\sqrt{\frac{\rho_p k_1}{D_e}}} - \frac{1}{s-\sqrt{\frac{\rho_p k_1}{D_e}}}\right]$$

$$\Rightarrow \cancel{\frac{dC}{ds}} \quad C = \frac{C_A(0)}{2\sqrt{\frac{\rho_p k_1}{D_e}}} \ln\left[\frac{s+\sqrt{\frac{\rho_p k_1}{D_e}}}{s-\sqrt{\frac{\rho_p k_1}{D_e}}}\right]$$

$$C = \frac{C_A(0)}{2\sqrt{\frac{S_p k_1}{D_e}}} \ln\left(\frac{s + \sqrt{\frac{S_p k_1}{D_e}}}{s - \sqrt{\frac{S_p k_1}{D_e}}}\right)$$

$$\mathcal{L}(C_A) = \frac{C_A(0)}{2\sqrt{\frac{S_p k_1}{D_e}}} \ln\left(\frac{s + \sqrt{\frac{S_p k_1}{D_e}}}{s - \sqrt{\frac{S_p k_1}{D_e}}}\right)$$

$$\Rightarrow C_A = \frac{C_A(0)}{2\sqrt{\frac{S_p k_1}{D_e}}} \; \frac{e^{\sqrt{\frac{S_p k_1}{D_e}}\, r} - e^{-\sqrt{\frac{S_p k_1}{D_e}}\, r}}{r}$$

So using boundary condition,

$$\Rightarrow C_{A,S} = \frac{C_A(0)}{2\sqrt{\frac{S_p k_1}{D_e}}} \; \frac{e^{\sqrt{\frac{S_p k_1}{D_e}}\, R} - e^{-\sqrt{\frac{S_p k_1}{D_e}}\, R}}{R}$$

$$\Rightarrow C_{A,S} = \frac{C_A(0)}{\sqrt{\frac{S_p k_1}{D_e}}} \; \frac{\sinh\left(\sqrt{\frac{S_p k_1}{D_e}}\, R\right)}{R}$$

So...

$$C_A(0) = C_{AS} \frac{(3\phi_s)}{\sinh(3\phi_s)}$$

$$\cancel{C_A = R / C_{A,S}}$$

$$\therefore C_A(r) = \frac{R\, C_{AS}}{\sinh\left(\sqrt{\frac{S_p k_1}{D_e}}\, R\right)} \cdot \frac{\sinh\left(\sqrt{\frac{S_p k_1}{D_e}}\, r\right)}{r}$$

$$\therefore \boxed{C_A(r) = C_{A,S}\left(\frac{R}{r}\right)\left[\frac{\sinh\left(\sqrt{\frac{S_p k_1}{D_e}}\, r\right)}{\sinh\left(\sqrt{\frac{S_p k_1}{D_e}}\, R\right)}\right]}$$

for 1st order reaction

$$\phi_s = \frac{R}{3}\sqrt{\frac{k_1 \rho_p}{D_e}}$$ = Thiele modulus for a spherical pellete.

$$\boxed{\frac{C_A}{C_{A,s}} = \frac{R}{r} \frac{\sinh\left(3\phi_s \frac{r}{R}\right)}{\sinh(3\phi_s)}}$$

Determimination of r_p:

rate of diffusion = rate of reaction in the pellet

$$\frac{\text{rate of reaction}}{\text{Unit weight of the catalyst. (W)}} = \frac{4\pi R^2 D_e \left(\frac{dC_A}{dr}\right)_{r=R}}{W}$$

$$r_p = \frac{4\pi R^2 D_e \left(\frac{dC_A}{dr}\right)_{r=R}}{\frac{4}{3}\pi R^3 \rho_p}$$

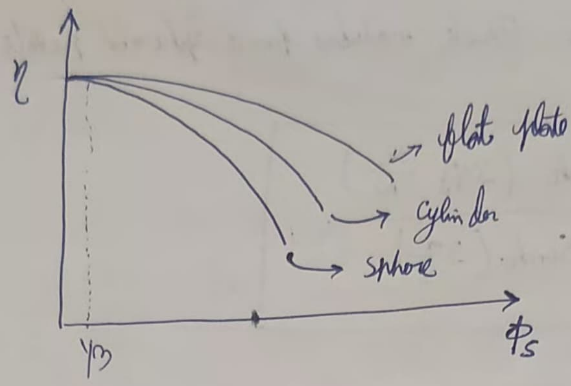
$$r_p = \frac{3}{R\rho_p} D_e \left(\frac{dC_A}{dr}\right)$$

Effectiveness factor (η):

$$\eta = \frac{r_p}{r_s} = \frac{\frac{3}{R\rho_p} D_e \frac{dC_A}{dr}}{k_1 C_{AS}}$$

where, $k_1 C_{AS}$ = rate of reaction on the surface of the catalyst particle $= r_s$

$$\therefore \eta = \frac{1}{\phi_s}\left[\frac{1}{\tanh(3\phi_s)} - \frac{1}{3\phi_s}\right]$$



$$\eta_f > \eta_{cy} > \eta_{sp} \text{ for a fixed } \phi_s$$

for sphere, Thiele modulus.

$$\phi_s = \frac{R}{3}\sqrt{\frac{k_1 \rho_p}{D_e}}$$

for non spherical,

$$\phi_s = 3\left(\frac{V_p}{S_p}\right) = R.$$

when, $\eta \sim 1$,

we neglect pore diffusion resistance, for this $\phi < 1$

Significance of Thiele modulus:

→

Determination of effectiveness factor η:

Bulk diffusivity

D_{AB}

Knudsen diffusivity

$D_K = 9700\, a \sqrt{\frac{T}{m}}$

$\longrightarrow$ effectiveness diffusivity

$D_e = \frac{\phi_p \sigma}{\tau} D$

Thiele modulus.

$\phi_s = \frac{R}{3} \sqrt{\frac{k_1 \rho_p}{D_e}}$

effectiveness factor

$\eta = \frac{1}{\phi_s}\left[\frac{1}{\tanh(3\phi_s)} - \frac{1}{3\phi_s}\right]$

Determination of effectiveness factor / Thiele modulus for reversible 1st order reaction:

$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$

$$-\frac{dC_A}{dt} = k_1 C_A - k_2 C_B \quad \text{.....} \; (i)$$

for constant volume and no mole change,

$$C_B = C_{B0} + (C_{A0} - C_A)$$

So now.

$$-\frac{dC_A}{dt} = k_1 C_A - k_2 (C_{B0} + C_{A0} - C_A)$$

$$= (k_1 + k_2) C_A - k_2 (C_{A0} + C_{B0})$$

now, at eqm, $k_1 C_{Aeq} = k_2 C_{Beq}$

$$K = \frac{C_{Beq}}{C_{Aeq}} = \frac{C_{B0} + (C_{A0} - C_{Aeq})}{C_{Aeq}}$$

So

$$-\frac{dC_A}{dt} = k_1 C_A + \frac{k_1}{K} C_A - \frac{k_1}{K}(C_{A0} + C_{B0})$$

$$= k_1\left[\left(1+\frac{1}{K}\right)C_A - \frac{1}{K}(C_{A0} + C_{B0})\right]$$

$$= k_1\left[\frac{K+1}{K} C_A - C_{Aeq}\,\frac{K+1}{K}\right]$$

$$-\frac{dC_A}{dt} = k_1\left(1+\frac{1}{K}\right)(C_A - C_{Aeq})$$

$$-\frac{dC_A}{dt} = K_R (C_A - C_{Aeq})$$ where

$$K_R = k_1\left(\frac{K+1}{K}\right)$$

$$C_A' = C_A - C_{Aeq}.$$

$$\therefore -\frac{dC_A'}{dt} = K_R C_A'$$

for reversible reaction mole balance,

$$\left(-4\pi r^2 D_e \frac{dC_A'}{dt}\right)_r - \left(-4\pi r^2 D_e \frac{dC_A'}{dr}\right)_{r+\Delta r} = 4\pi r^2 \Delta r\, \rho_p K_R C_A'$$

So.

$$\cancel{\frac{d}{dr}\left(4\pi r^2 D_e \frac{dC_A'}{dr}\right) = \rho_p K_R C_A'}$$

$$\cancel{\therefore D_e \frac{d^2 C_A'}{dr'^2} = \rho_p K_R C_A'}$$

$$\frac{d^2 C_A'}{dr^2} + \frac{2}{r}\frac{dC_A'}{dr} - \frac{K_R \rho_P C_A'}{D_e} = 0$$

$\frac{dC_A}{dr} = 0$ at, $r = 0$ and, $C' = C_s'$, $r = R$

So. $\phi_s' = \frac{R}{3}\sqrt{\frac{K_R \rho_p}{D_e}}$

$\therefore$ $$\boxed{\phi_s' = \frac{R}{3}\sqrt{\frac{k_1(K+1)\rho_p}{K D_e}}}$$

→ Thiele modulus for reversible reaction is more than that of irreversible reaction by a factor of $\sqrt{\left(1+\frac{1}{K}\right)}$.

→ $C_{Ab} \approx C_{AS}$

$\eta \to 1$ $\quad$ r_p we can get from

↳ $r_p = r_s$

$\phi_s \leq \frac{1}{3} \Rightarrow \eta \to 1$ (experimentally)

$$\frac{R}{3}\sqrt{\frac{\rho_p k_1}{D_e}} \leq \frac{1}{3}$$

$$R\sqrt{\frac{\rho_p k_1}{D_e}} \leq 1$$

$$\frac{R^2 \rho_p k_1}{D_e} \leq 1$$

r_p = rate of the reaction within the catalyst (considering $C_s \simeq C_A$) and $C_s \simeq C_{Ab}$ ~~sub~~ neglecting external diffusional resistance)

$r_p = k_1 C_A$. $\therefore k_1 = \frac{r_p}{C_A}$.

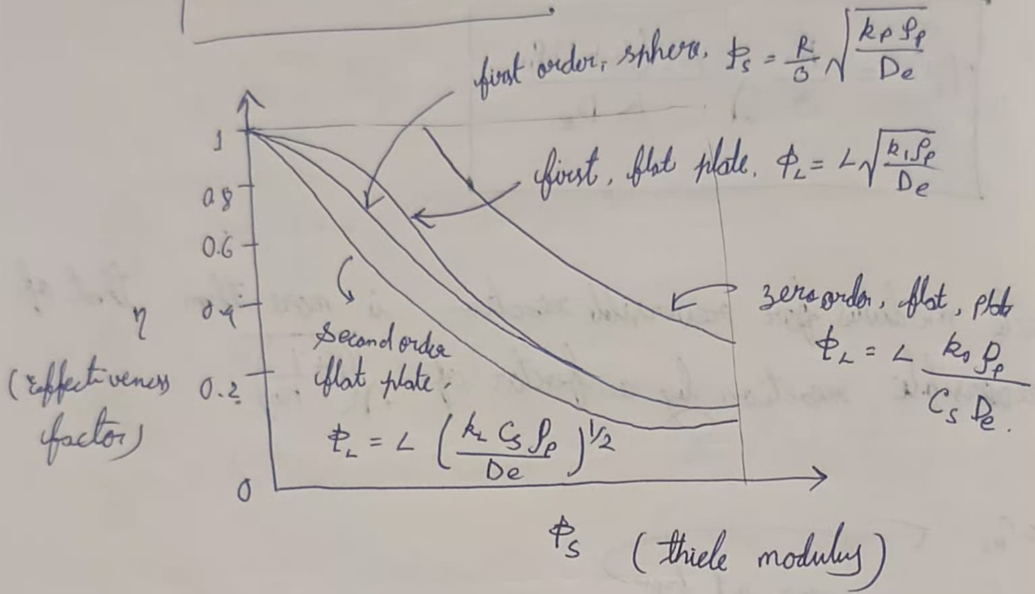
So, $$\boxed{R^2 \frac{r_p \rho_p}{C_A D_e} \leq 1}$$

$$\boxed{C_{WP} \leq 1}$$

when there is almost no pore diffusional resistance: $C_{WP} \le 1$

C_{WP} = Weisz and Prater Criterion

$$\boxed{C_{WP} = R^2 \frac{r_p \rho_p}{C_A D_e}}$$



Q. Dehydrogenation of butane using chromia-Alumina catalyst at 530°C is done. For a spherical catalyst of size $d_p = 0.32$ cm. The exp. data suggests a first order rate constant of 0.94 $cm^3/g.s$

The pore radius is given as 110 Å. Assuming Knudsen diffusion at low pressure and estimating the pore volume 0.35 cm^3/g, predict an effectiveness factor for the catalyst. Use a parallel pore model with a $\tau = 3$.

Ans.

$$\eta = \frac{1}{\phi_s}\left[\frac{1}{\tanh(3\phi_s)} - \frac{1}{3\phi_s}\right]$$

$$\phi_s = \frac{R}{3}\sqrt{\frac{k_1 \rho_p}{D_e}}$$

C_4H_{10}

$D_k = 9700\, a\sqrt{\frac{T}{M}}$

$= 9700 \times 110\times10^{-8} \times \sqrt{\frac{803}{58}}$

$= 0.0397\ cm^2/s.$

$D_e = \frac{\phi_p \sigma}{\tau} D_k$

$\phi_p = \rho_p V_g$

So $\cancel{\phi_s = \frac{0.16}{3}\sqrt{\frac{0.34\times\frac{1}{0.35}}{0.0397}}\sqrt{\frac{\tau}{\phi_p\sigma}} = 0.439\sqrt{\frac{\tau}{\phi_p\sigma}}}$

So

$\phi_p = 0.35\rho_p.$

So $D_e = \frac{0.35\rho_p}{3}\times 0.0397.$

So $\phi_s = \frac{R}{3}\sqrt{\frac{k_1 \cancel{\rho_p}}{\frac{0.35\cancel{\rho_p}}{3}\times 0.0397}}$

$\Rightarrow \phi_s = \frac{0.16}{3}\sqrt{\frac{0.34\times 3}{0.35\times 0.0397}}$

$\therefore \phi_s = 0.759$ & $3\phi_s = 2.277.$

So $\eta = \frac{1}{\phi_s}\left[\frac{1}{\tanh(3\phi_s)} - \frac{1}{3\phi_s}\right]$

now $\tanh(3\phi_s) = \frac{2}{1+e^{-4.554}} - 1 = 0.979$

$\Rightarrow \eta = \frac{1}{0.759}\left(\frac{1}{0.979} - \frac{1}{2.277}\right)$

$\therefore \boxed{\eta = 0.767}$

Evaluation of effectiveness factor η, when internal diffusional resistance exists :

Two sized spherical catallyst pellet,

R_1 and R_2.

corresponding effectiveness factor η_1 and η_2 and Thiele modulus ϕ_{S_1} and ϕ_{S_2}, rate of the reactions r_1 and r_2 respectively,

k_1 = rate constant for the particular reaction.

ρ_P and D_e are taken constant.

$$r_1 = k_1 C_A \eta_1 \quad , \quad r_2 = k_1 C_A \eta_2.$$

$$\eta_1 = \frac{1}{\phi_{S_1}} \left[\frac{1}{\tanh(3\phi_{S_1})} - \frac{1}{3\phi_{S_1}} \right]$$

$$\eta_2 = \frac{1}{\phi_{S_2}} \left[\frac{1}{\tanh(3\phi_{S_2})} - \frac{1}{3\phi_{S_2}} \right]$$

$$\phi_{S_1} = \frac{R_1}{3}\sqrt{\frac{k_1 \rho_P}{D_e}} \quad , \quad \phi_{S_2} = \frac{R_2}{3}\sqrt{\frac{k_1 \rho_P}{D_e}}$$

$$\frac{\phi_{S_2}}{\phi_{S_1}} = \frac{R_2}{R_1}$$

unknowns are, $\eta_1, \eta_2, \phi_{S_1}, \phi_{S_2}$

$$\frac{r_2}{r_1} = \frac{\eta_2}{\eta_1} \quad , \quad \frac{\phi_{S_2}}{\phi_{S_1}} = \frac{R_2}{R_1}$$

Mass and heat transfer with reaction, Effectiveness factor:

$\eta = \dfrac{\text{actual rate of the reaction in the pellet}}{\text{rate of the reaction on the surface of the pellet}}$

$\eta = \dfrac{r_p}{r_s}$

$\therefore r_p = r_s \eta = \eta f(T_s, C_s)$

non-isothermal effectiveness factor

Non-isothermal effectiveness factor:

for isothermal effectiveness factor, considering only mass transfer.

$$\left(-4\pi r^2 D_e \frac{dC}{dr}\right)_r - \left(-4\pi r^2 D_e \frac{dC}{dr}\right)_{r+\Delta r} = 4\pi r^2 \Delta r \, \rho_p k_1 C$$

B.C

(i) $\left.\dfrac{dC}{dr}\right|_{r=0} = 0$ at, $r = 0$.

(ii) $C = C_s$ at, $r = R$.

$$\frac{d^2 C}{dr^2} + \frac{2}{r}\frac{dC}{dr} - \frac{\rho_p k_1}{D_e} C = 0$$

$$\therefore D_e\left(\frac{d^2C}{dr^2} + \frac{2}{r}\frac{dC}{dr}\right) = k_1 \rho_p C \quad \dots (1)$$

for heat transfer, Energy Balance.

$$\left(-4\pi r^2 K_e \frac{dT}{dr}\right)_r - \left(-4\pi r^2 K_e \frac{dT}{dr}\right)_{r+\Delta r} = 4\pi r^2 \Delta r \rho_p k_1 C \Delta H$$

K_e = effective ~~...~~ thermal diffusivity.

ΔH = heat of the reaction.

Taking $\Delta r \to 0$

we get,

$$\frac{d^2T}{dr^2} + \frac{2}{r}\frac{dT}{dr} - \frac{\rho_p \Delta H k_1 C}{K_e} = 0$$

BC.

$$\left.\frac{dT}{dr}\right|_{r=0} = 0 \quad , \quad T = T_s \text{ when, } r = R.$$

So.

$$\frac{K_e}{\Delta H}\left(\frac{d^2T}{dr^2} + \frac{2}{r}\frac{dT}{dr}\right) = k_1 \rho_p C.$$

now comparing we get;

$$\frac{K_e}{\Delta H}\left(\frac{d^2T}{dr^2} + \frac{2}{r}\frac{dT}{dr}\right) = D_e\left(\frac{d^2C}{dr^2} + \frac{2}{r}\frac{dC}{dr}\right)$$

we get;

$$(T - T_s) = \frac{\Delta H D_e}{K_e}(C - C_s)$$

when, $C=0$, i.e, maximum rate, (rate of the reaction = rate of diffusi

$$(T - T_s)_{max} = -\frac{\Delta H D_e}{K_e} C_s$$

Three dimensionless factors on which η depends:

i) Thiele modulus.

$$3(\phi_s)_s = R\sqrt{\frac{(k_1)_s \rho_p}{D_e}}$$

$(\phi_s)_s$ = Thiele modulus at T_s

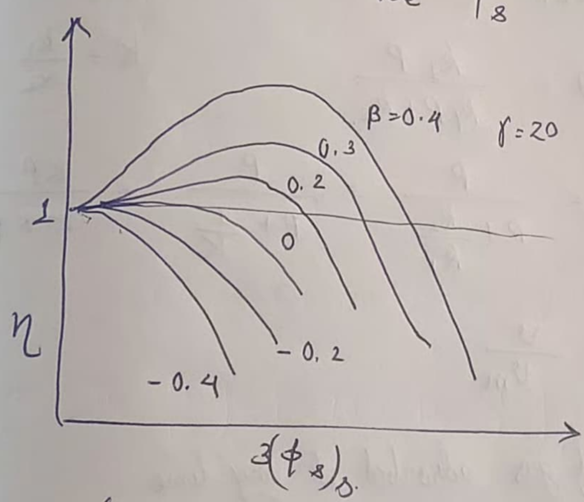
$(k_1)_s$ = rate constant at T_s.

ii) Arrhenius number:

$$\gamma = \frac{E}{R_g T_s}$$

(iii) Heat of reaction parameter.

$$\beta = \frac{(-\Delta H) D_e C_s}{K_e T_s}$$



$\beta +$ → exothermic.

$\beta -$ → endothermic

β 0 → isothermal.

Physical Significance:

i) For endothermic reaction, T ↓ so Rate of reaction decreases.

ii) For exothermic reaction T ↑ so.