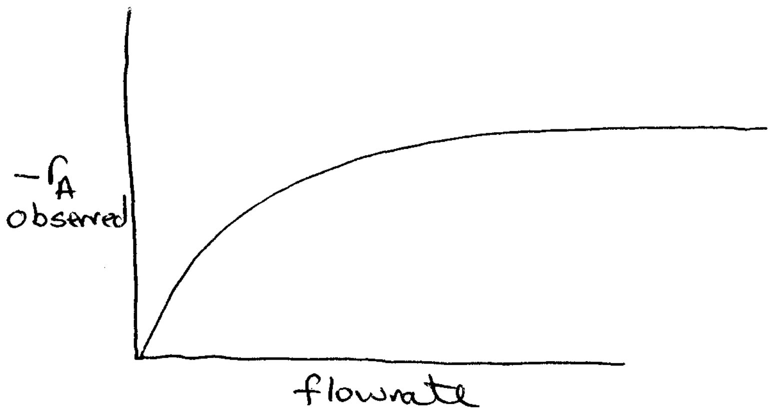
Chapter 11 External Effects



What is happening ?

- Catalytic reaction

looking at the entire sphere:
(catalyst particle)

$$W_{Ar} = k_c\left(C_{A\,bulk} - C_{A\,surface}\right)$$

$$Sh = \frac{k_c d_p}{D_{AB}} \qquad Sc = \frac{\nu}{D_{AB}} = \frac{\mu/\rho}{D_{AB}} \qquad \frac{\text{kinematic viscosity}}{\text{Diffusivity}}$$

$$Sh = 2 + 0.6\,Re^{1/2}\,Sc^{1/3}$$ — Frossling Correlation fo

See next page for packed bed

Example 10-4 Rapid reaction at catalyst surface $C_{As} = 0$?

(Measure reaction rate)

C_{Ab}

C_{As}

$$W_{Ar} = k_c\left(C_{Ab} - C_{As}\right) = \underbrace{k_r}_{\left(\frac{mol}{s\,m^3_{cat}}\right)\frac{m^3\text{cat volume}}{m^2\text{cat surface}}} \overbrace{C_{As}}^{\text{surface reaction Rate}} = r_{surface} \qquad \left\{ r = \frac{mol}{s\,m^2} \right.$$

$$k_c C_{Ab} - k_c C_{As} = k_r C_{As}$$

How do you measure C_{As} ?

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

Rapid Reaction $k_r >> k_c$ {mass transfer limited}

$$C_{As} = \frac{k_c C_{Ao}}{k_r} \rightarrow 0$$

Slow reaction

$k_c >> k_r$

$C_{As} = C_{Ab}$

ignore mass transfer

$$r_{surface} = \underset{\infty}{\underset{\uparrow}{k_r}}\ \underset{0}{\underset{\uparrow}{C_{As}}} = k_c\left(C_{Ab} - 0\right) = k_c C_{Ab}$$

Reaction rate vs external mass transfer

$$k_c(C_{Ab}-C_{As}) = W_A\Big|_{\text{surface}} = \Theta r_A' = k_s' C_{As} = \left[\frac{k_s \rho_c}{S}\right] C_{As}$$

$$\frac{\rho_c k_s}{S} = \left(\frac{L}{s\ \text{kg cat}}\right)\left(\frac{\text{kg cat}}{m^3\ \text{cat}}\right)\left(\frac{1}{m^2\ \text{cat}/m^3\ \text{cat}}\right)$$

$$C_{As} = \frac{k_c C_{Ab}}{k_c + k_s'}$$

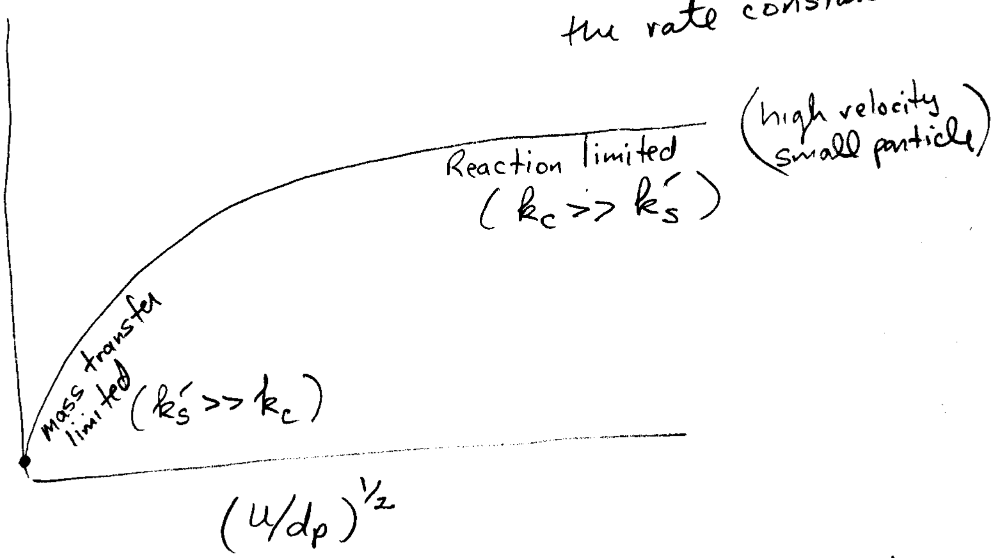
"old" k measured from reaction rate data.

Bulk conc.

$$-r_A' = \underline{\underline{k_s' C_A}} = k_s' C_{As} = k_s'\left[\frac{k_c C_{Ab}}{k_c + k_s'}\right] = \left[\frac{k_s' k_c}{k_c + k_s'}\right] C_{Ab}$$

So we were ok using the global definition, but now we have some knowledge of the rate constant!

$$-r_A' = \frac{k_s' k_c}{k_c + k_s'} C_{Ab}$$



$$\frac{3/6 \quad 2/6}{}\qquad \frac{\rho^{1/2}\,\rho^{-1/3}\,\mathcal{D}_{AB}}{\mu^{1/2}\,\mu^{-1/3}\,\mathcal{D}_{AB}^{-1/3}} \Rightarrow \frac{\rho^{1/6}\,\mathcal{D}_{AB}^{2/3}}{\mu^{1/6}}$$

$$\mu^{-3/6}\mu^{2/6} \Rightarrow \mu^{-1/6}$$

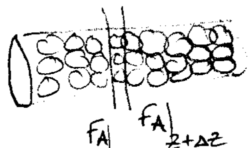
$$\frac{k_c d_p}{\mathcal{D}_{AM}} = 2 + 0.6\left[\frac{\rho U d_p}{\mu}\right]^{1/2}\left[\frac{\mu/\rho}{\mathcal{D}_{AM}}\right]^{1/3} \Rightarrow k_c = 2\frac{\mathcal{D}_{AM}}{d_p} + 0.6\left[\frac{U}{d_p}\right]^{1/2}\left(\frac{\rho}{\mu}\right)^{1/6}\mathcal{D}_{AM}^{2/3}$$

$$Sh = 2 + 0.6\, Re_p^{1/2}\, Sc^{1/3}$$

Complete the picture

Mass transfer in a packed-bed

mole balance on A



$$r_s' \;[=]\; \frac{mol}{s\, m^2_{\text{cat surface}}}$$

$$0 = F_A\big|_z - F_{A_{z+\Delta z}} + r_A A_c \Delta z \qquad r = r_s' a \qquad a \;[=]\; \frac{m^2_{cat}}{m^3_{Bed}}$$

$$\frac{dF_A}{dz} = r_A A_c = r_{A_s}' a A_c$$

Neglecting diffusion in the axial direction – fast flows

In z-direction

$$F_{A_z} = \underset{\substack{\uparrow \\ \frac{mol}{s\, m^2_{Bed}}}}{W_{A_z}} A_c = \Big[\underbrace{\cancel{J_{A_z}}}_{\text{small}} + y_A (W_{A_z} + W_{B_z})\Big] A_c = \underset{\frac{mol}{m^3}}{C_{A_b}} \varphi$$

for φ = constant

$$\frac{\varphi}{A_c} \frac{dC_{A_b}}{dz} = r_{A_s}' a$$

$$r_{A_s}' = -k C_{A_s}$$

$$u \frac{dC_{A_b}}{dz} = r_{A_s}' a \qquad \text{two choices} \qquad -r_{A_s}' = W_{A_z} = k_c (C_{A_b} - C_{A_s})$$

$$-r_{A_s}' = \left[\frac{k_s' k_c}{k_c + k_s'}\right] C_{A_b}$$

$$u\frac{dC_{Ab}}{dz} = -\left[\frac{k_s' k_c a}{k_c + k_s'}\right] C_{Ab}$$

Integrating $\quad \ln C_{Ab} = -\frac{1}{u}\left[\frac{k_s' k_c a}{k_c + k_s'}\right] z + k_1$

Initial condition $z = 0 \quad C_{Ab} = C_{Ab0} \qquad K_1 = \ln C_{Ab0}$

$$\ln\left[C_{Ab}/C_{Ab0}\right] = -\left[\frac{k_s' k_c a}{k_c + k_s'}\right] z/u$$

$$\frac{C_{Ab}}{C_{Ab0}} = \exp\left[-\left[\frac{k_s' k_c a}{k_c + k_s'}\right]\frac{z}{u}\right]$$

$$k_c = \left(\frac{u}{d_p}\right)^{1/2} D_{AB}^{2/3} \left(\frac{\rho}{\mu}\right)^{1/6}$$

limiting cases $\quad k_c >> k_s \qquad\qquad k_s >> k_c$

$$\frac{C_{Ab}}{C_{Ab0}} = \exp\left[-\left(k_s' a \frac{z}{u}\right)\right] \qquad\qquad \frac{C_{Ab}}{C_{Ab0}} = \exp\left[-k_c a \frac{z}{u}\right]$$

section 10.3.4
10.3.3

Single sphere – Frossling equation

Packed Bed (many spheres) ⇒ Thoenes and Kramers

$$Sh' = (Re')^{1/2} Sc^{1/3}$$

equation <u>10-66</u>

void fraction

$0.25 < \epsilon_b < 0.5$

$40 < Re' < 4000$

$1 < Sc < 4000$

$$k_c \propto \left(\frac{u}{d_p}\right)^{1/2}$$