10.37 Chemical and Biological Reaction Engineering, Spring 2007
Prof. William H. Green

Lecture 21: Reaction and Diffusion in Porous Catalyst (cont'd)

This lecture covers: Packed bed reactors

$$\frac{dF_A}{dz} = Ar_{A_{eff}}$$

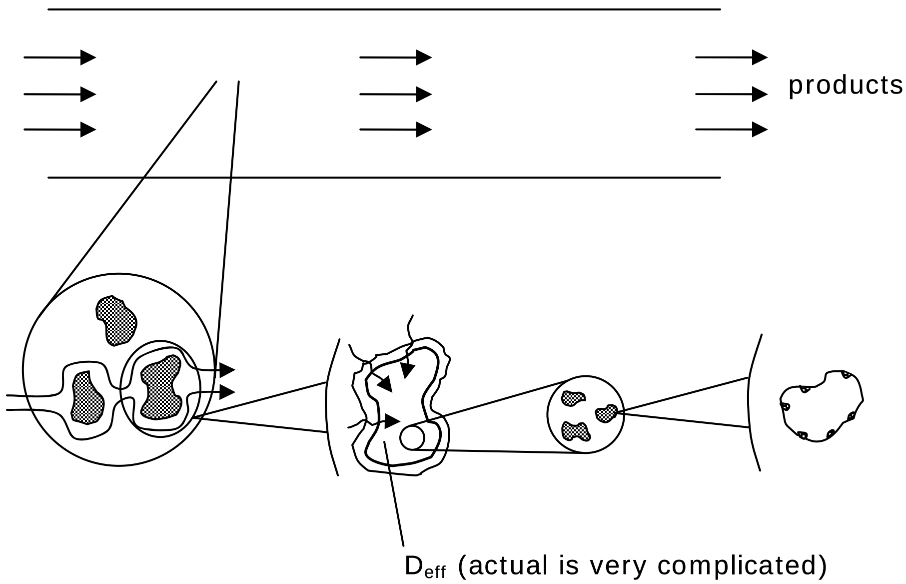

Figure 1. Packed Bed Reactor

Void Fraction $\phi \sim .5$

$$\underbrace{\begin{matrix} C_A(x_j, y_m, z_l) \\ j=1,30 \\ m=1,30 \\ l=1,30 \end{matrix}}_{\text{(points)}}$$

(11-21) $D_i \nabla^2 C_i - \underline{U} \cdot \nabla C_i + r_i^{fluid} = 0$ ← in the fluid i=1, $N_{species}{}^{fluid}$

$$D_i \left. \frac{\partial C_i}{\partial \hat{n}} \right|_{surface} + r_i^{surface} = 0$$ (boundary condition for the above)

Ergun's Eq.:

(4-22) $$\frac{dP}{dz} = -\frac{G}{\rho g_c D_p} \frac{1-\phi}{\phi^3} \left[\frac{150(1-\phi)\mu}{D_p} + 1.75G \right]$$

where $P = \rho RT$, $\rho U_z = \frac{G}{A}$

$$\frac{\partial F_A}{\partial z} = A r_A^{eff}$$

area

$$r_A^{eff} = (\text{effectiveness factor}) r_A C_{A_b}(z)$$

$\Omega\left(C_{A_b}(z)\right)$ (or η internal)

total

$$\Omega \equiv \frac{\text{Actual rate of reaction } (r_A^{eff})}{\text{Rate if } C_A = C_{A_{bulk}}(z), \text{ and } T = T_{bulk} \text{ everywhere}}$$

$$\frac{\partial F_i}{\partial z} = A r_i^{eff} = A \Omega r_i^{ideal} \qquad r_i^{ideal} [=] \frac{\text{mol}}{\text{vol. s}}$$

$$r_i^{ideal} = r_i' \left(\frac{\text{wt. of catalyst in reactor}}{\text{V reactor}} \right)$$

$$\begin{aligned} r_i &= r_i' \rho_c (1-\phi) \\ &= r_i'' \left(\frac{\text{surface area of cat.}}{\text{wt. cat.}} \right) \rho_c (1-\phi) \end{aligned}$$

$$a_c / m_{particle}$$

$$\frac{m^2}{g} [=] S_a + (\text{macroscopic surface area, visual})$$

$$F_A = \nu C_A = A U C_A \quad \text{(some approximation)}$$

Dispersion

$$\frac{1}{A}\frac{dF_A}{dz} = +U \frac{dC_A}{dz} - \cancel{D_a \frac{d^2 C_A}{dz^2}}$$

hope this is 0!

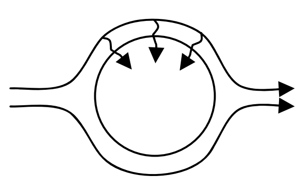

Figure 2. Flow over a sphere

$$k_c a_c\left(C_{A_b} - C_{As}\right) = \eta\left(C_{As}\right) r_A^{\,particle}\left(C_{As}\right) V_p$$

$$D_{inside}\frac{\partial^2 C_A}{\partial r^2} + r_A\left(C_A(r)\right) = 0$$

$$\left.\frac{\partial C_A}{\partial r}\right|_{r=0} = 0 \qquad\qquad D_{eff\ inside}\frac{\partial C_A}{\partial r} = k_c\left(C_{A_b} - C_{As}\right)$$

$$k_c C_A\big|_{r=R} + D_{eff\ inside}\left.\frac{\partial C_A}{\partial r}\right|_{r=R} = k_c C_{A\,bulk}$$

Matlab:

1) Guess C_{As} (C_A surface)
2) Use boundary conditions to get corresponding $\left.\frac{\partial C_A}{\partial r}\right|_{r=R}$
3) Solve ODE (ode15s)
4) Vary guess (C_{As}) to make $\frac{\partial C_A}{\partial r} = 0$ at center

1[st] oder irrev.

$$\Omega = \frac{\eta}{1 + \dfrac{\eta k_1'' S_a \rho_b}{k_c a_c}} \qquad\qquad \eta = \frac{3}{\phi_1^2}\left(\phi_1 \coth(\phi_i) - 1\right)$$

$$\phi_1 = \ldots\sqrt{k_1''}$$