

LECTURE ELEVEN: Packed bed reactors.

This lecture covers: Packed bed reactors

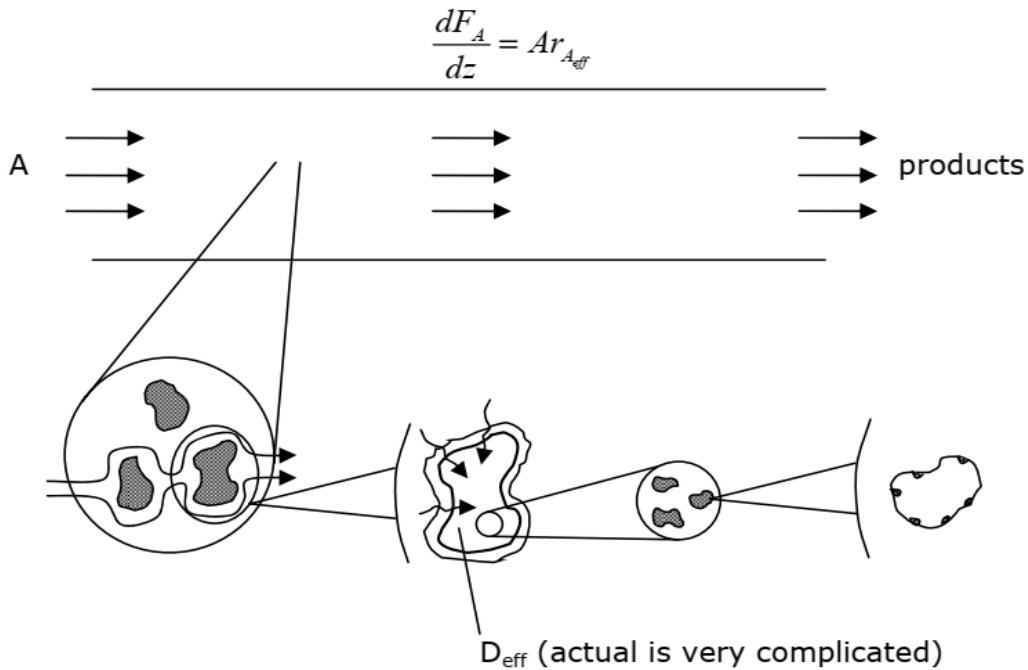


Figure 1. Packed Bed Reactor

Void Fraction $\phi \sim .5$

$$C_A(x_j, y_m, z_l)$$

$$j = 1, 30$$

$$m = 1, 30$$

$$l = 1, 30$$

(points)

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

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

Ergun's Eq.:

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

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

$$\frac{\partial F_A}{\partial z} = A r_A^{eff} \quad r_A^{eff} = (\text{effectiveness factor}) r_A C_{A_b}(z)$$

↑
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↑

area
 $\Omega(C_{A_b}(z))$ (or η internal)
total

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

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

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

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

$$a_c / m_{particle}$$

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

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

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

↙ Dispersion
hope this is 0!

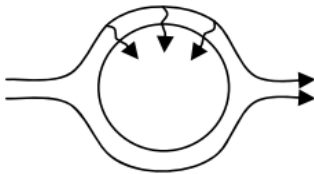


Figure 2. Flow over a sphere

$$k_c a_c (C_{A_b} - C_{A_s}) = \eta (C_{A_s}) r_A^{particle} (C_{A_s}) V_p$$

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

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

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

Matlab:

- 1) Guess C_{A_s} (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_{A_s}) to make $\left. \frac{\partial C_A}{\partial r} \right|_{r=0} = 0$ at center

1st oder irrev.

$$\Omega = \frac{\eta}{1 + \frac{\eta k_1'' S_a \rho_b}{k_c a_c}}$$

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

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