

Homework 11 - Solutions

1. The reaction $A \rightarrow B$ is taking place in a PBR at a pressure of 2 atmospheres and a temperature of 500 K. Pure A enters the reactor packed with catalyst spheres of 10 mm diameter at a molar rate of 2 mol/s. The diffusion coefficient is $0.25 \text{ cm}^2/\text{s}$. The rate is given by $r'_A = 6 C_A \frac{\text{mol}}{(\text{kg-cat})\text{-s}}$. The bulk density of the catalyst is 2.6667 kg/lit. What is the conversion when the bed is packed with 10 kg of the catalyst? What is the percentage decrease in conversion due to internal diffusion?

35 points

$$\phi = R \sqrt{\frac{k \rho}{D}} = 0.5 \sqrt{\frac{6 \cdot 2.6667}{0.25}} = 4$$

$$\eta = \frac{3}{\phi^2} \left(\frac{\phi}{\tanh \phi} - 1 \right) = 0.563$$

$$F_{A0} \frac{dX}{dW} = -r'_A = k C_A = \eta k C_{A0} (1 - X)$$

$$= \eta k C_{A0} (1 - X)$$

$$\frac{dX}{dW} = \frac{\eta k C_{A0}}{F_{A0}} (1 - X)$$

$$\int_0^X \frac{1}{1 - X} dX = \frac{\eta k}{v_0} \int_0^W dW$$

$$\ln \frac{1}{(1 - X)} = \frac{\eta k}{v_0} W$$

$$v_0 = 41 \frac{\text{l}}{\text{s}}, k = 6, \eta = 0.563$$

$$W = 10 \text{ kg}$$

$$X = 0.5613$$

No internal diffusion - $\eta=1$

$$X = 0.7686$$

Percentage reduction in X due to internal diffusion = 27%

2. t-Butyl alcohol is produced by the liquid-phase hydration of isobutene. Water reacts with isobutene over an Amberlyst-15 catalyst. The reactions are:

Adsorption of isobutene (I): $I + S \rightleftharpoons I \cdot S$

Adsorption of water (W): $W + S \rightleftharpoons W \cdot S$

Surface Reaction: $I \cdot S + W \cdot S \rightleftharpoons TBA \cdot S + S$

Desorption of t-butyl alcohol (TBA): $TBA \cdot S \rightleftharpoons TBA + S$

- Write down the rates of all the individual reactions.
- Obtain the concentrations of intermediates assuming that the surface reaction is the rate controlling step.
- Substitute the concentrations from step b into the surface reaction rate and obtain the final form of the rate expression by performing a site balance.

Additional information:

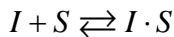
$$K_p = \frac{K_s K_I K_W}{K_{TBA}}$$

K_s = Surface reaction equilibrium constant

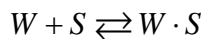
K_I = Adsorption equilibrium constant for I

K_W = Adsorption equilibrium constant for W

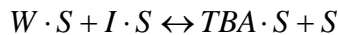
K_{TBA} = Adsorption equilibrium constant for TBA



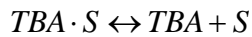
$$r_{ADI} = k_{AI} \left[C_I C_V - \frac{C_{I \cdot S}}{K_I} \right]$$



$$r_{ADI} = k_{AW} \left[C_W C_V - \frac{C_{W \cdot S}}{K_W} \right]$$



$$r_s = k_s \left[C_{W \cdot S} C_{I \cdot S} - \frac{C_V C_{TBA \cdot S}}{K_s} \right]$$



$$r_D = K_D \left[C_{TBA \cdot S} - \frac{C_{TBA} C_V}{K_D} \right]$$

3. A first-order, gas-phase reaction $A \rightarrow 2B$ is performed in a PBR at 400 K and 10 atm. Feed rate is 5 mol/s containing 20% A and the rest inerts. The PBR is packed with 8 mm-diameter spherical porous particles. The intrinsic reaction rate is given as:

$r'_A = 3.75 C_A$ mol/kg(cat)-s. Bulk density of the catalyst is 2.3 kg/liter. The diffusivity is 0.1 cm²/s. The pressure drop parameter alpha is found to be 9.8×10^{-4} kg⁻¹.

- What is the value of the internal effectiveness factor? What does it signify?

- b. How much catalyst (kg) is required to obtain a conversion of 75% in the reactor?
 c. Find the pressure at the exit of the reactor.

$$\phi = R\sqrt{\frac{k\rho}{D}} = 0.4\sqrt{\frac{3.75 \cdot 2.3}{0.1}} = 3.714$$

$$\eta = \frac{3}{\phi^2} \left(\frac{\phi}{\tanh \phi} - 1 \right) = 0.5912$$

$$F_{A0} \frac{dX}{dW} = -r'_A = kC_A = \eta k C_{A0} \frac{(1-X) P}{(1+\varepsilon X) P_0}$$

$$= \eta k C_{A0} \frac{(1-X)}{(1+\varepsilon X)} (1-\alpha W)^{1/2}$$

$$\frac{dX}{dW} = \frac{\eta k C_{A0}}{F_{A0}} \frac{(1-X)}{(1+\varepsilon X)} (1-\alpha W)^{1/2}$$

$$\int_0^X \frac{1+\varepsilon X}{1-X} dX = \frac{\eta k}{v_0} \int_0^W (1-\alpha W)^{1/2} dW$$

$$(1+\varepsilon) \ln \frac{1}{(1-X)} - \varepsilon X = \frac{\eta k}{v_0} \frac{2}{3\alpha} \left[1 - (1-\alpha W)^{3/2} \right]$$

$$v_0 = 16.4 \text{ lit/s}; X = 0.75; \varepsilon = 0.2; \alpha = 9.8 \times 10^{-4}; \eta = 0.5912;$$

$$k = 3.75$$

$$W = 11.22 \text{ kg}$$

$$\frac{P}{P_0} = (1-\alpha W)^{1/2} = 0.9944$$

$$P = 9.94 \text{ atm}$$

4. A residence time distribution (in terms of reduced time = $\left(\frac{t}{\bar{t}}\right) = \theta$) is given by:

$$E(\theta) = 15\theta^2 \exp(-2.5\theta)$$

Mean residence time is 3. The reaction is first order with a rate constant of 0.5 in consistent units. Find the conversion with the given RTD and segregated flow and compare it to conversions from a PFR and a CSTR. Comment on your results. Additional information.

$$\int_0^{\infty} ax^2 \exp(-bx) dx = \frac{2a}{b^3}$$

5. CDP 13-M from your text.