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 cm^2/s. The rate is given by $r_A' = 6C_A \dfrac{\text{mol}}{\text{(kg-cat)-s}}$. 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

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

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

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

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

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

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

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

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

$$W = 10\ kg$$

$$X = 0.5613$$

No internal diffusion - η=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): $I + S \rightleftarrows I{\bullet}S$

Adsorption of water (W): $W + S \rightleftarrows W{\bullet}S$

Surface Reaction: $I{\bullet}S + W{\bullet}S \rightleftarrows TBA{\bullet}S + S$

Desorption of t-butyl alcohol (TBA): $TBA{\bullet}S \rightleftarrows TBA + S$

a. Write down the rates of all the individual reactions.
b. Obtain the concentrations of intermediates assuming that the surface reaction is the rate controlling step.
c. 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

$$I + S \rightleftarrows I \cdot S$$

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

$$W + S \rightleftarrows W \cdot S$$

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

$$W \cdot S + I \cdot S \leftrightarrow TBA \cdot S + S$$

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

$$TBA \cdot S \leftrightarrow TBA + S$$

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

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 cm^2/s. The pressure drop parameter alpha is found to be 9.8×10^{-4} kg^{-1}.
   a. 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.

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

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

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

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

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

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

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

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

$$k = 3.75$$

$$W = 11.22\ kg$$

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

$$P = 9.94\ atm$$

4. A residence time distribution (in terms of reduced time = $\left(\frac{t}{\bar{t}}\right)$ = θ) 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.