Quiz 5 Solutions

CHBE 424

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1. (10 pts) Gaseous reactant A diffuses through a gas film and reacts on the surface of a solid according to a reversible first-order rate, $-r''_A = k''(C_{As} - C_{Ae})$ where C_{Ae} is the concentration of A in equilibrium with the solid surface, and C_{As} is the concentration of A on the solid surface. Develop an expression for the overall rate of reaction of A accounting for both the mass transfer and reaction steps in terms of C_{Ab}, C_{Ae}, k'', and k_c, where C_A is the concentration of A in the bulk phase, and k_c is the mass transfer coefficient.

Problem 1 Solution

From mass transfer flux,

$W_{Ar} = k_c(C_{Ab} - C_{As})$

From the surface reaction,

$-r''_{AS} = k''(C_{As} - C_{Ae})$

At steady-state, $W_{Ar} = -r''_{As}$

Hence, $k_c(C_{Ab} - C_{As}) = k''(C_{As} - C_{Ae})$

$\Rightarrow k_c C_{Ab} + k'' C_{Ae} = (k'' + k_c) C_{As}$

$\Rightarrow C_{As} = \dfrac{k_c C_{Ab} + k'' C_{Ae}}{k'' + k_c}$

Hence, the overall rate is given as

$-r''_{As} = k''(C_{As} - C_{Ae}) = k'' \left(\dfrac{k_c C_{Ab} + k'' C_{Ae}}{k'' + k_c} - C_{Ae} \right)$

$$\boxed{-r''_{As} = \frac{k'' k_c}{k'' + k_c}(C_{Ab} - C_{Ae})}$$

2. (15 pts) The growth of germanium by chemical vapor deposition occurs according to the following series of reactions:

	Equilibrium Constant
$GeCl_{2(g)} + S \xleftrightarrow{\text{k}_1} GeCl_2 \cdot S$	K_1
$H_{2(g)} + 2S \xleftrightarrow{\text{k}_1} 2(H \cdot S)$	K_2
$GeCl_2 \cdot S + 2(H \cdot S) \xrightarrow{\text{k}_3} Ge_{(s)} + 2HCL + 3S$	

The surface reaction is rate-limiting. Derive the rate expression for Ge deposition in terms of partial pressures of $GeCl_2$ and H_2, specific rate constants, and the equilibrium constants.

Problem 2 Solution

Since the surface reaction is rate limiting,

$r_{Ge} = k_3[GeCl_2{\cdot}S][H{\cdot}S]^2$

Assuming the other two reactions are at equilibrium,

$$[GeCl_2{\cdot}S] = K_1 P_{GeCl_2} \cdot C_v \tag{1}$$

$[H{\cdot}S]^2 = K_2 P_{H_2} \cdot C_v^2$

$$\Rightarrow H{\cdot}S = \sqrt{K_2 P_{H_2}} \cdot C_v \tag{2}$$

From the catalyst site blanace,

$C_v + [H{\cdot}S] + [GeCl_2{\cdot}S] = C_T$

$\Rightarrow C_v + \sqrt{K_2 P_{H_2}} \cdot C_v + K_1 P_{GeCl_2} \cdot C_v = C_T$

$$\Rightarrow C_v = \frac{C_T}{1 + \sqrt{K_2 P_{H_2}} + K_1 P_{GeCl_2}} \tag{3}$$

Plug in expressions from (1) and (2) into the rate equation,

$r_{Ge} = k_3[GeCl_2{\cdot}S][H{\cdot}S]^2 = k_3 K_1 K_2 P_{GeCl_2} P_{H_2} \cdot C_v^3$

Plug in C_v from (3)

$$\boxed{r_{Ge} = k_3 K_1 K_2 P_{GeCl_2} P_{H_2} \left[\frac{C_T}{1 + K_1 P_{GeCl_2} + \sqrt{K_2 P_{H_2}}}\right]^3}$$

3. (25 pts) The zero-order reaction $A \to B$ is carried out in a moving bed reactor containing 1 kg of catalyst. The catalyst decay is also zero-order. The entering molar flow rate is pure A at 1 mol/min. Given the following information: (1) The product sells from \$160 per gram mole. (2) The cost of operating the bed is \$10 per kilogram of catalyst exiting the bed. (3) The specific reaction rate: $k_r = 1.0$ mol/kg catalyst $\cdot$ min, and the decay consstant: k_d 2.0 min^{-1}.

(a) Write catalyst activity and conversion in terms of catalyst weight, respectively.
(b) What is the feed rate of solids (kg/min) that will give the maximum profit?
(c) What are the catalyst activity and conversion exiting the reactor at this optimum?

Hint: For the purpose of this calculation, ignore all other costs, such as the cost of reactant, etc. Write the equation for the profit in terms of feed rate of solids and find the maximum profit analytically.

Problem 3 Solution

(a)

catalyst activity, a follows zero-order rate law:

$$\frac{da}{dt} = -k_d; \;\; dt = \frac{dw}{U_s} \Rightarrow \frac{da}{dw} = -\frac{k_d}{U_s}$$

$$\int_1^a da = -\frac{k_d}{U_s}\int_0^w dw$$

$$\Rightarrow \boxed{a = 1 - \frac{k_d}{U_s} \cdot w}$$

Mole balance: $\dfrac{dX_A}{dw} = \dfrac{-r'_A}{F_{A0}}$

Rate law: $-r'_A = k_r a = \left(1 - \dfrac{K_d}{U_s} w\right) k_r$

$$\frac{dX_A}{dw} = \frac{k_r}{F_{A0}}\left(1 - \frac{k_d w}{U_s}\right)$$

Integrate:

$$\int_0^{X_A} dX_A = \frac{k_r}{F_{A0}}\int_0^w \left(1 - \frac{k_d w}{U_s}\right) dw$$

$$\boxed{X_A = \frac{k_r}{F_{A0}}\left(w - \frac{k_d w^2}{2U_s}\right)}$$

(b)

Profit = (Selling price of final product) - (Cost of catalyst flow)

$P = 160 F_{A0} X_A - 10 U_s$

To maximize P w.r.t. U_s; $\quad \dfrac{dP}{dU_s} = 0$

$$\frac{dP}{U_s} = \frac{d}{dU_s}(160F_{A0}X_A - 10U_s) = 160F_{A0}\frac{dX_A}{dU_s} - 10 = 0$$

$$\frac{dX_A}{U_s} = \frac{d}{dU_s}\left(\frac{k_r}{F_{A0}}\left(w - \frac{k_d}{2U_s}w^2\right)\right) = \frac{k_r k_d w^2}{2F_{A0}U_s^2}$$

$$\frac{dP}{dU_s} = 160F_{A0}\left(\frac{k_r k_d w^2}{2F_{A0}U_s^2}\right) - 10 = 0$$

Solve for U_s; $\quad U_s = \sqrt{8k_r k_d}$

$$w = \sqrt{8 \cdot 1 \cdot 2}(1)\frac{kg}{min} = 4\frac{kg}{min}$$

$$\boxed{U_s = 4\frac{kg}{min}}$$

(c)

$$X_A = \frac{k_r}{F_{A0}}\left(w - \frac{k_d w^2}{2U_s}\right) = \frac{1}{1}\left(1 - \frac{2 \cdot 1^2}{2 \cdot 4}\right) = 0.75$$

$$\boxed{X_A = 0.75}$$

$$a = 1 - \frac{k_d}{U_s}w = 1 - \frac{2}{4} \cdot 1 = 0.50$$

$$\boxed{a = 0.50}$$