CRE HOMEWORK #8

PROBLEM #1

$$I + S \rightleftharpoons I \cdot S$$

$$W + S \rightleftharpoons W \cdot S$$

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

$$TBA \cdot S \rightleftharpoons TBA + S$$

$$r_1 = k_1 (I)(S) - k_{-1} (I \cdot S)$$

$$r_1 = k_1 \left[(I)(S) - \frac{(I \cdot S)}{K_1} \right]$$

$$r_2 = k_2 \left[(W)(S) - \frac{(W \cdot S)}{K_2} \right]$$

$$r_3 = k_3 \frac{(W \cdot S)(I \cdot S)}{C_t} - \frac{k_{-3} (TBA \cdot S)(S)}{C_t}$$

$$r_3 = k_3 \left[\frac{(W \cdot S)(I \cdot S)}{C_t} - \frac{(TBA \cdot S)(S)}{C_t K_3} \right]$$

$$r_4 = k_4 \left[(TBA \cdot S) - \frac{(TBA)(S)}{K_4} \right]$$

1,2,4 ARE QE

$$K_1 (I)(S) = (I \cdot S) \qquad K_2 (W)(S) = (W \cdot S)$$

$$(TBA \cdot S) = \frac{(TBA)(S)}{K_4}$$

$$C_t = (S) + (I \cdot S) + (W \cdot S) + (TBA \cdot S)$$

$$C_t = (S) + K_1(I)(S) + K_2(W)(S) + \frac{(TBA)(S)}{K_4}$$

$$K_4 = \frac{1}{K_{TBA}}$$

$$(S) = \frac{C_t}{K_1(I) + K_2(W) + K_{TBA}(TBA) + 1}$$

$$r_3 = k_3\left[\frac{K_1 K_2 (I)(W)(S)^2}{C_t} - \frac{K_{TBA}(TBA)(S)^2}{K_3 C_t}\right]$$

$$r_3 = \frac{k_3 C_t\left[K_1 K_2 (I)(W) - \frac{K_{TBA}(TBA)}{K_3}\right]}{\left[1 + K_1(I) + K_2(W) + K_{TBA}(TBA)\right]^2}$$

$$r_I = r_3$$

b. $-r_I = r_1 = k_1\left((I)(S) - \frac{(I\cdot S)}{K_1}\right)$

Step #3 is QE

$$k_3\frac{(W\cdot S)(I\cdot S)}{C_t} = k_{-3}\frac{(TBA\cdot S)(S)}{C_t}$$

$$(I\cdot S) = \frac{(TBA\cdot S)(S)}{(W\cdot S)K_3}$$

$$-r_I = k_1\left[(I)(S) - \frac{(TBA\cdot S)(S)}{(W\cdot S)K_3K_1}\right]$$

$$-r_I = k_1\left[(I)(S) - \frac{(TBA\cdot S)(S)(S)}{K_2K_3K_1(S)(W\cdot S)}\right]$$

$$C_t = (S) + (I\cdot S) + (W\cdot S) + (TBA\cdot S)$$

$$C_t = (S) + \frac{K_{TBA}(TBA)(S)}{K_2K_3(W)} + K_2(W)(S)$$

$$+ K_{TBA}(TBA)(S)$$

$$(S) = \frac{C_t}{1 + \frac{K_{TBA}(TBA)}{K_2K_3(W)} + K_2(W) + K_{TBA}(TBA)}$$

$$-r_I = k_1 \left[\frac{(I)\, c_t}{1 + \frac{K_{TBA}(TBA)}{K_2 K_3 (W)} + K_2(W) + K_{TBA}(TBA)} - \frac{K_{TBA}(TBA)\, c_t}{K_1 K_2 K_3 (W) \left[1 + \frac{K_{TBA}(TBA)}{K_2 K_3 (W)} + K_2(W) + K_{TBA}(TBA) \right]} \right]$$

$$I + S \rightleftharpoons I \cdot S$$

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

$$TBA \cdot S \rightleftharpoons TBA + S$$

$$r_2 = k_2 (I \cdot S)(W) - k_{-2} (TBA \cdot S)$$

$$r_2 = k_2 K_1 (I)(S)(W) - k_{-2} K_{TBA} (TBA)(S)$$

$$r_2 = k_2 \left(K_1 (I)(S)(W) - \frac{K_{TBA}(TBA)(S)}{K_2} \right)$$

$$c_t = (S) + (I \cdot S) + (TBA \cdot S)$$

$$c_t = (S) \left[1 + K_1 (I) + K_{TBA}(TBA) \right]$$

$$-r_I = r_2 = \frac{k_2 \left[K_1 c_t (I)(W) - \frac{K_{TBA}(TBA)\, c_t}{K_2} \right]}{1 + K_1 (I) + K_{TBA}(TBA)}$$

d. $I + S_1 \rightleftharpoons I \cdot S_1$

$W + S_2 \rightleftharpoons W \cdot S_2$

$I \cdot S_1 + W \cdot S_2 \rightleftharpoons TBA + S_1 + S_2$

$$r_3 = k_3 (I \cdot S_1)(W \cdot S_2) - k_{-3} (TBA)(S_1)(S_2)$$

QE ON STEPS 1 + 2

$$(I \cdot S_1) = K_1 (I)(S_1)$$

$$(W \cdot S_2) = K_2 (W)(S_2)$$

$$C_{t,1} = (S_1) + (I \cdot S_1) = S_1 (1 + K_1 (I))$$

$$C_{t,2} = (S_2)(1 + K_2 (W))$$

$$r_3 = k_3 \left[(I \cdot S_1)(W \cdot S_2) - \frac{(TBA)(S_1)(S_2)}{K_3} \right]$$

$$r_3 = k_3 \left[\frac{K_1 (I) C_{t,1}}{(1 + K_1 (I))} \frac{K_2 (W) C_{t,2}}{(1 + K_2 (W))} - \frac{(TBA) C_{t,1} C_{t,2}}{K_3 (1 + K_1 (I))(1 + K_2 (W))} \right]$$

PROBLEM #2

a. $-r'_{AS} = k' C_{AS}$

$$\frac{dF_A}{dW} = -r'_{AS}$$

$$F_{A0}\frac{dX_A}{dW} = -r'_{AS} = k' C_{AS}$$

$$F_{A0} = C_{A0} v_0 = \left(\frac{1\ \text{mol}}{L}\right)\left(\frac{10\ L}{s}\right) = \frac{10\ \text{mol}\ A}{s}$$

ASSUMING MASS TRANSFER LIMITATIONS

$$W_A = k_c (C_A - C_{AS})$$

$$C_{AS} = \frac{k'_c C_A}{k'_c + k'}$$

$$Sh = 100\sqrt{Re}$$

$$k_c = \frac{D_{AB}}{d_p} Sh = \frac{D_{AB}}{d_p}(100)\sqrt{\rho v d_p/\mu}$$

$$k_c = 70.7\ \text{cm/s}$$

$$k'_c = k_c \alpha = (70.7\ \text{cm/s})\left(\frac{60\ \text{cm}^2}{g\ \text{cat}}\right) = 4242\ \frac{\text{cm}^3}{g\ \text{cat}\cdot s}$$

$$C_A = C_{A0}(1-X)$$

$$\frac{dX}{dW} = \frac{-r'_{AS}}{F_{A0}} = \frac{C_{A0}(1-X_A)k' k'_c}{F_{A0}(k' + k'_c)}$$

$$\int_0^{0.6} \frac{dX}{1-X} = W \cdot \frac{C_{A0}}{F_{A0}} \frac{k' k_c'}{k' + k_c'}$$

$$\boxed{W = 916 \text{ kg}}$$

b. non-isothermal adiabatic

$$k'(T) = k'(300K) \exp\left[\frac{E_A}{R} \left(\frac{1}{300K} - \frac{1}{T} \right) \right]$$

$$C_A = C_{A0}(1-X)\left(\frac{T_0}{T}\right)$$

MASS BALANCE:

$$\frac{dX}{dW} = \frac{r_{AS}'}{F_{A0}}$$

ENERGY BALANCE

$$T + T_0 - \frac{\Delta H_R X}{\sum \Theta_i c_{pi}} = 300K + \frac{10000 \frac{cal}{mol} X}{100 \frac{cal}{mol \cdot K}}$$

COMBINE MASS + ENERGY BALANCES

$$\frac{dX}{dW} = \frac{T_0}{T} \frac{C_{A0}(1-X_A)}{F_{A0}} \frac{k' k_c'}{k_c' + k_A'}$$

$$\boxed{W = 538 \text{ kg}}$$