CHFEN 3553
Chemical Reaction Engineering

Heat Effects

$$\frac{dE}{dt} = \overset{0}{Q} - \overset{0}{W} + \sum_{1=1}^{n} F_{i0} H_{i0} - \sum_{i=1}^{n} F_{ie} H_{ie}$$

Define

$$\Delta H_{Rx}(T) = \frac{d}{a} H_D + \frac{c}{a} H_C - \frac{b}{a} H_B - H_A$$

$$\frac{dE}{dt} = \overset{0}{Q} - \overset{0}{W} - F_{A0} \sum_{i=1}^{n} \theta_i (H_i - H_{i0}) - \Delta H_{Rx}(T) \cdot F_{A0} \cdot X = 0$$

Most general energy balance that can be used even when phase change is taking place.

Simplifications when no phase change is involved

Enthalpy at any temperature T is the sum of the enthalpy at reference temperature and sensible heat (only when there is no phase change)

$$H(T) = H(T_R) + \Delta H_Q$$

$$\Delta H_Q = \int_{T_1}^{T_2} C_{pi}\, dT$$

$$H_i - H_{i0} = \int_{Ti0}^{T_i} C_{pi}\, dT$$

Substituting in the heat balance equation

$$\overset{0}{\dot{Q}} - \overset{0}{\dot{W}} - F_{A0}\sum_{i=1}^{n}\theta_i \int_{Ti0}^{T_i} C_{pi}dT - \Delta H_{Rx}(T)\cdot F_{A0}\cdot X = 0$$

Heat of reaction at temperature T is related to the reference temperature Tr by (This is derived using the same sensible heat relationship)

$$\Delta H_{Rx}(T) = \Delta H_{Rx}(T_R) + \int_{T_R}^{T} \Delta C_p dT$$

$$\Delta C_p = \frac{d}{a}C_{pD} + \frac{c}{a}C_{pC} - \frac{b}{a}C_{pB} - C_{pA}$$

Specific heat relationships are polynomials which can be substituted into the integral relationships.

Simplification of the integral involving Cp

$$\int_{T_R}^{T} \Delta C_p dT = \Delta\hat{C}_p (T - T_R)$$

$$\int_{T_{i0}}^{T} \Delta C_p dT = \tilde{C}_p (T - T_{i0})$$

Values of Qdot.

CSTR: $\dot{Q} = U \cdot A \cdot (T_a - T)$

If the temperature in the jacket can be approximated to be constant.

U – Overall heat transfer coefficient = energy/time-area-K

A – Total heat exchange area

PFR:

$$\dot{Q} = \int_V U \cdot a \cdot (T_a - T)\, dV$$

$$\frac{d\dot{Q}}{dV} = U \cdot a \cdot (T_a - T)$$

$$a = \frac{\pi D h}{\pi D^2 / 4h} = \frac{4}{D}$$

a=Heat exchange area per unit volume

$$\frac{d\dot{Q}}{dW} = \frac{U \cdot a}{\rho_b}(T_a - T)$$

Summary of Heat Balance Relationships

Most General

With phase changes

$$\overset{0}{Q} - \overset{0}{W} - F_{A0}\sum_{i=1}^{n}\theta_i (H_i - H_{i0}) - \Delta H_{Rx}(T)\cdot F_{A0}\cdot X = 0$$

Without phase change

$$\overset{0}{Q} - \overset{0}{W} - F_{A0}\sum_{i=1}^{n}\theta_i \int_{Ti0}^{T_i} C_{pi}dT - \Delta H_{Rx}(T)\cdot F_{A0}\cdot X = 0$$

$$\overset{0}{Q} - \overset{0}{W} - F_{A0}\sum_{i=1}^{n}\theta_i \int_{Ti0}^{T_i} C_{pi}dT - [\Delta H_{Rx}(T_R) + \int_{T_R}^{T} \Delta C_p dT]\cdot F_{A0}\cdot X = 0$$

$$\overset{0}{Q} - \overset{0}{W} - F_{A0}\sum_{i=1}^{n}\theta_i \tilde{C}_p (T - T_{i0}) - [\Delta H_{Rx}(T_R) + \Delta \hat{C}_p (T - T_R)]\cdot F_{A0}\cdot X = 0$$

Combining the energy balance and the material balances

Material balance

$$V = \frac{F_{A0}X}{-r_A}$$

$$\frac{\dot{Q}-\dot{W}}{F_{A0}} - X\left[\Delta H_{Rx}(T_R) + \Delta\hat{C}_p(T - T_R)\right] = \sum_{i=1}^{n}\theta_i\tilde{C}_p(T - T_{i0})$$

$$\dot{Q} = U \cdot A \cdot (T_a - T)$$

$$If\ \dot{W} = 0\ \ and\ \Delta C_p = 0 \cdots only\ A\ entering$$

$$T = \frac{F_{A0}X(-\Delta H^0_{Rx}) + F_{A0}\tilde{C}_{pA}T_0 + U \cdot A \cdot T_a}{F_{A0}\tilde{C}_{pA} + U \cdot A}$$

Adiabatic Operation

$$T = \frac{X(-\Delta H^0_{Rx})}{\tilde{C}_{pA}} + T_0$$

Table 8-4 Page 443 – Study Please ……

V specified – solve for X and T

X specified – solve for V and T

T specified – solve for X and V

Additional Relationships

$$-r_A = kC_A$$

$$k = Ae^{\frac{-E}{RT}}$$

PFR Balances

Mole Balance

$$F_{A0}\frac{dX}{dV} = -r_A(X,T)$$

$$X(-\Delta H_{Rx}(T)) = \int_{T_{i0}}^{T}\sum \theta_i C_{pi} dT$$ For adiabatic operation

Tubular reactor with heat exchange

Differentiate the energy balance equation with respect to V

$$\dot{Q} - F_{A0}\int_{T_0}^{T}\sum \theta_i C_{pi} dT - F_{A0}X\left[\Delta H_{Rx}^{0}(T_R) + \int_{T_R}^{T}\Delta C_p dT\right] = 0$$

Simplification and regrouping yields

$$\frac{dT}{dV} = \frac{U \cdot a \cdot (T_a - T) + \left[(-r_A)\cdot(-\Delta H_{Rx}(T)\right]}{F_{A0}\left(\sum \theta_i C_{pi} + X\Delta C_p\right)}$$