PHEN 612

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WEEK 5

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Chapter 8
Steady-state Non-isothermal Reactor Design

8.1 In addition to the Arrhenius equation, we need to understand how the temperature affects the conversion X.

8.2 Energy Balance

- First law (closed system): $$d\hat{E} = \delta Q - \delta W$$
- First law (open system): $$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W} + F_{in}E_{in} - F_{out}E_{out}$$
- The first law for open systems can be extended to several inlet and outlet flows.
- These equations help to understand the influence of heat on a system operating isothermally

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8.2.2 The work term ($\dot{W}$) accounts for flow work (due to materials crossing the boundary) and shaft work (e.g., stirrer in a CSTR, turbine in a PFR):

$$\dot{W} = \sum_{i=1}^{n} F_i P\tilde{V}_i \bigg|_{out} - \sum_{i=1}^{n} F_i P\tilde{V}_i \bigg|_{in} + \dot{W}_s$$

By using $H_i = U_i + P\tilde{V}_i$ and neglecting the contribution of potential and internal energies

$$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_{i0} H_{i0} - \sum_{i=1}^{n} F_i H_i$$

- F: is the molar flow rate; H: specific molar enthalpy; V: specific molar volume; P: the pressure; U: internal energy

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8.2.3 We need to develop relationship between system temperature, conversion, molar flow rate and system parameters.

8.2.4 We know that heat of reaction plays a significant role in reaction engineering. How do we integrate the heat of reaction in the heat transfer equation?

<u>Steady-state consideration:</u> accumulation rate = 0

$$0 = \dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_{i0} H_{i0} - \sum_{i=1}^{n} F_i H_i$$

The reaction is given by: A + (b/a)B -> (c/a)C + (d/a)D

Using: $\sum_{i=1}^{n} F_i H_i = F_A H_A + F_B H_B + F_C H_C + F_D H_D + F_I H_I$ for the inlet and outlet flows

and $F_i = F_{A0}\left(\Theta_i + \nu_i X\right)$ we have

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8.2.5

$$\dot{Q} - \dot{W}_s + F_{A0}\sum_{i=1}^{n}\Theta_i\left(H_{i0} - H_i\right) - \Delta H_{RX}\left\langle T\right\rangle F_{A0}X = 0$$

with the heat of reaction defined as:

$$\Delta H_{RX}\left\langle T\right\rangle = \frac{d}{a}H_D\left\langle T\right\rangle + \frac{c}{a}H_C\left\langle T\right\rangle - \frac{b}{a}H_B\left\langle T\right\rangle - H_A\left\langle T\right\rangle$$

For a process with no phase change and constant heat capacity C_p, we have

$$H_i - H_{i0} = C_{pi}\left(T - T_{i0}\right)$$

As a result:

$$\dot{Q} - \dot{W}_s - F_{A0}\sum_{i=1}^{n}\Theta_i C_{pi}\left(T_i - T_{i0}\right) - \Delta H_{RX}\left\langle T\right\rangle F_{A0}X = 0$$

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8.2.6

- If we use a reference condition (R):

$$\Delta H_{RX}\langle T\rangle = \Delta H_{RX}^{0}\langle T_R\rangle + \Delta C_p\left(T - T_R\right)$$

we have (for no shaft work):

$$\dot{Q} - F_{A0}\sum_{i=1}^{n}\Theta_i C_{pi}\left(T_i - T_{i0}\right) - \left[\Delta H_{RX}^{0}\langle T_R\rangle + \Delta C_p\left(T - T_R\right)\right]F_{A0}X = 0$$

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8.4 Steady-state tubular reactor with heat exchanger.

In this case:

$$\Delta\dot{Q} = U\Delta A\left(T_a - T\right) = Ua\left(T_a - T\right)\Delta V$$

- Where Ta is the ambient temperature, T, the reactor temperature, and U, the overall heat transfer coefficient. The heat exchanger area is give by a: a = A/V = 4/D

- With no shaft work and taking into account the design equation:

$$\frac{dF_i}{dV} = r_i = \nu_i\left(-r_A\right)$$

Heat generated

Heat removed

We have: $$\frac{dT}{dV} = \frac{r_A \Delta H_{RX} - Ua\left(T_a - T\right)}{\sum F_i C_{pi}}$$

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In terms of conversion X

$$\frac{dT}{dV}=\frac{r_A\Delta H_{RX}-Ua\left(T_a-T\right)}{F_{A0}\left(\sum\Theta_i C_{pi}+\Delta C_p X\right)}$$

- For packed-bed:

$$\frac{dT}{dW}=\frac{r_A^{'}\Delta H_{RX}-\frac{Ua}{\rho_b}\left(T_a-T\right)}{\sum F_i C_{pi}}$$

8.4.2 Balance on the coolant heat transfer fluid (c)

Co-current flow: $$\frac{dT_a}{dV}=\frac{Ua\left(T-T_a\right)}{\dot{m}_c C_{Pc}}$$

Counter-current flow: $$\frac{dT_a}{dV}=\frac{Ua\left(T_a-T\right)}{\dot{m}_c C_{Pc}}$$