PHEN 612

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WEEK 6

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Chapter 9
Unsteady Steady-state Non-isothermal Reactor Design

- 9.1 Unsteady-state Energy Balance $$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W}_s + \sum F_i H_i \Big|_{in} - \sum F_i H_i \Big|_{out}$$

- The total energy can be written in terms of energies associated with the reactants, products, and inert:

$$\hat{E}_{sys} = \sum_{i=1}^{n} N_i E_i = N_A E_A + N_B E_B + N_C E_C + N_D E_D + N_I E_I$$

- If we neglect potential and kinetic energies:

$$\hat{E}_{sys} = \sum_{i=1}^{n} N_i U_i = \sum_{i=1}^{n} N_i \left(H_i - PV_i\right)\Big|_{sys} = \left[\sum_{i=1}^{n} N_i H_i - \sum_{i=1}^{n} \left(PV_i\right)\right]_{sys} = \left[\sum_{i=1}^{n} N_i H_i - \underline{P\sum_{i=1}^{n} \left(N_i \tilde{V}_i\right)}\right]_{sys}$$

V

PV

- If PV is small compared to $\sum_{i=1}^{n} N_i H_i$

$$\dot{Q} - \dot{W}_s + \sum F_i H_i \Big|_{in} - \sum F_i H_i \Big|_{out} = \left[\sum N_i \frac{dH_i}{dt} + \sum H_i \frac{dN_i}{dt}\right]_{sys}$$

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Using $H_i = H_i^0 \langle T_R \rangle + \int_{T_R}^{T} C_{pi} dT$ <u>Species: i</u>

we have: $$\dot{Q} - \dot{W}_s + \sum F_i H_i \Big|_{in} - \sum F_i H_i \Big|_{out} = \left[\sum N_i C_{pi} \frac{dT}{dt} + \sum H_i \frac{dN_i}{dt} \right]_{sys}$$

or

$$\dot{Q} - \dot{W}_s + \sum F_{i0} H_{i0} - \sum F_i H_i = \sum N_i C_{pi} \frac{dT}{dt} + \sum H_i \frac{dN_i}{dt}$$

- The mole balance is: $\frac{dN_i}{dt} = F_{i0} - F_i - \nu_i r_A V$

Also $\sum \nu_i H_i = \Delta H_{RX}$ $\Longrightarrow$ $$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum F_{i0} \left(H_i - H_{i0} \right) + \left(-\Delta H_{RX} \right) \left(-r_A V \right)}{\sum N_i C_{pi}}$$

No phase change

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum F_{i0} C_{pi} \left(T - T_{i0} \right) + \left(-\Delta H_{RX} \langle T \rangle \right) \left(-r_A V \right)}{\sum N_i C_{pi}}$$

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For liquid phase reactions (where ΔC_p small):

$$\sum_{i=1}^{n} N_i C_{pi} \cong \sum_{i=1}^{n} N_{i0} C_{pi} = N_{A0} \sum_{i=1}^{n} \Theta_i C_{pi} = N_{A0} C_{ps}$$

where C_{ps} is the heat capacity of the solution

Similarly $$\sum_{i=1}^{n} F_{i0} C_{pi} = F_{A0} C_{ps}$$

Then $$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - F_{A0} C_{ps} \left(T - T_{i0}\right) + \left(-\Delta H_{RX} \left\langle T \right\rangle\right)\left(-r_A V\right)}{N_{A0} C_{ps}}$$

9.2 Energy Balance on Batch Reactors: $$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s + \left(-\Delta H_{RX} \left\langle T \right\rangle\right)\left(-r_A V\right)}{\sum_{i=1}^{n} N_i C_{pi}}$$

In terms of conversion X: $$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s + \left(-\Delta H_{RX} \left\langle T \right\rangle\right)\left(-r_A V\right)}{N_{A0} \left(\sum_{i=1}^{n} \Theta_i C_{pi} + \Delta C_p X \right)}$$

and $$N_{A0} \frac{dX}{dt}_i = -r_A V$$

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9.2.1 Adiabatic Operation of a Batch Reactor

$$\dot{Q} = 0; \quad F_{i0} = 0; \quad \dot{W}_s = 0$$

We have:

$$\frac{dT}{dt} = \frac{\left(-\Delta H_{RX}\left\langle T \right\rangle\right)\left(-r_A V\right)}{\sum_{i=1}^{n} N_i C_{pi}}$$

Conversion:

$$X = \frac{C_{ps}\left(T - T_0\right)}{\left(-\Delta H_{RX}\left\langle T \right\rangle\right)} = \frac{\sum \Theta_i C_{pi}\left(T - T_0\right)}{\left(-\Delta H_{RX}\left\langle T \right\rangle\right)}$$

$$T = T_0 + \frac{\left(-\Delta H_{RX}\left\langle T_0 \right\rangle\right) X}{C_{ps} + X \Delta C_p}$$

$$T = T_0 + \frac{\left(-\Delta H_{RX}\left\langle T_0 \right\rangle\right) X}{\sum_{i=1}^{n} N_i C_{pi} + X \Delta C_p}$$