

PHEN 612

SPRING 2008

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:

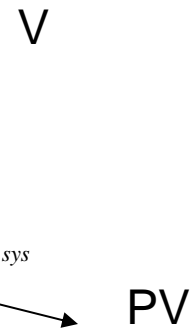
$$\hat{E}_{sys} = \sum_{i=1}^n N_i E_i = N_A E_A + N_B E_B + N_C E_C + N_D E_D + N_I E_I$$

- If we neglect potential and kinetic energies:

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

- 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 $H_i = H_i^0 \langle T_R \rangle + \int_{T_R}^T C_{pi} dT$ Species: i

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: $\frac{dN_i}{dt} = F_{i0} - F_i - v_i r_A V$

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

No phase change

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

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

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

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

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

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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:

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

Conversion:

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

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

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