9.5 Energy Balances on Reactive Processes

9.5a General Procedures

To perform energy balance calculations on a reactive system, proceed much as you did for non reactive system.

(a) draw and label a flowchart

(b) Use material balances and phase equilibrium relationships such as Raoult's law to determine as many ~~as~~ stream component amounts or flow rates as possible

(c) Choose reference states for specific enthalpy (or internal energy) calculations and prepare and fill in an inlet-outlet enthalpy or (internal energy) table.

(d) Calculate ΔH (or ΔU & ΔH), substitute the calculated value in the appropriate form of the energy balance equation, and complete the required calculation.

* Two methods are commonly used to choose reference states for enthalpy calculations and to calculate specific enthalpies and ΔH

A) Heat of Reaction Method

This method is generally preferable when there is a single reaction for which $\Delta \hat{H}_r^{\circ}$ is known.

(1) complete the material balance calculations on the reactor to the greatest extent possible.

(2) Choose reference states for specific enthalpy calculations.
reactant & product species at 25°c & 1atm
nonreacting species at any convenient temperature, such as the reactor inlet or outlet temperature or the reference condition used for the species in an available enthalpy table

(3) for a single reaction in a continuous process, Calculate the extent of reaction, $\dot{\xi}$, from Equation 9.1-3

$$\dot{\xi} = \frac{|\dot{n}_{A,out} - \dot{n}_{A,in}|}{|\nu_A|} = \frac{\dot{n}_{A,r}}{|\nu_A|}$$

(4) Prepare the inlet--outlet enthalpy table, inserting known molar amounts (n_i), or flow rates ($\dot{n}_i$) for all inlet and outlet stream components.

* If any of the components is at its reference state, insert 0 for the corresponding $\hat{H}_i$.

(5) Calculate each unknown stream component enthalpy, $\hat{H}_i$ as $\Delta\hat{H}$ for the species going from its reference state to the process state, and insert the enthalpies in the Table.

(6) Calculate $\Delta\dot{H}$ for the reactor

$$\Delta\dot{H} = \dot{\xi}\,\Delta\hat{H}_r^\circ + \sum \dot{n}_{out}\hat{H}_{out} - \sum \dot{n}_{in}\hat{H}_{in} \quad \text{(single reaction) 9.5-1a}$$

$$\Delta\dot{H} = \sum_{\text{reactions}} \dot{\xi}\,\Delta\hat{H}_{rj}^\circ + \sum \dot{n}_{out}\hat{H}_{out} - \sum \dot{n}_{in}\hat{H}_{in} \quad \text{(multiple reactions) 9.5-1b}$$

(7) Substitute the calculated value of $\Delta\dot{H}$ in the energy balance

$$\dot{Q} - \dot{W}_s = \Delta\dot{H} + \Delta\dot{E}_k + \Delta\dot{E}_p$$

B) Heat of Formation Method

This method is generally preferable for multiple reactions and single reactions for which $\Delta \hat{H}_r$ is not readily available

(1) Complete the material balance Calculations on the reactor to the greatest extend possible

(2) Choose reference states for enthalpy Calculations.

* This is the step that distinguishes the preceding method from this one.

The choices should be the elemental species that constitute the reactants and products in the states in which the elements are found at 25°C & 1atm and nonreacting species at any convenient temperature.

(3) Prepare the inlet-outlet enthalpy table.

(4) Calculate each unknown specific enthalpy.

(5) Calculate $\Delta \dot{H}$ for the reactor

$$\Delta \dot{H} = \sum \dot{n}_{out} \hat{H}_{out} - \sum \dot{n}_{in} \hat{H}_{in}$$

(6) Substitute the calculated value of $\Delta \dot{H}$ in the energy balance equation and complete the required calculations.