

There are two principal methods for calculating enthalpy changes associated with reactions. The first is to calculate the heat of reaction ($\Delta\hat{H}_r^\circ$) and extent of reaction (ξ) for each reaction. The reference states are the pure *compounds* at the reference temperatures and pressures. The first law then becomes:

First Law for Steady-State Reactive Systems (no shaft work)

$$\sum_{\text{out streams}} \left(\dot{n}_i + \sum_k \nu_{ik} \dot{\xi}_k \right) \hat{H}_j - \sum_{\text{in streams}} \dot{n}_i \hat{H}_i + \sum_{\text{rxns}} \dot{\xi}_k (\Delta\hat{H}_r^\circ)_k = \dot{Q}$$

Or implicitly accounting for the change in number of moles

$$\sum_{\text{out streams}} \dot{n}_j \hat{H}_j - \sum_{\text{in streams}} \dot{n}_i \hat{H}_i + \sum_{\text{rxns}} \dot{\xi}_k (\Delta\hat{H}_r^\circ)_k = \dot{Q}$$

For batch systems at constant pressure

$$\sum_{\text{final}} \left(n_i + \sum_k \nu_{ik} \xi_k \right) \hat{H}_j - \sum_{\text{initial}} n_i \hat{H}_i + \sum_{\text{rxns}} \xi_k (\Delta\hat{H}_r^\circ)_k = Q$$

Or implicitly accounting for the change in number of moles

$$\sum_{\text{final}} n_j \hat{H}_j - \sum_{\text{initial}} n_i \hat{H}_i + \sum_{\text{rxns}} \xi_k (\Delta \hat{H}_r^\circ)_k = Q$$

For batch systems at constant volume

$$\sum_{\text{final}} \left(n_i + \sum_k \nu_{ik} \xi_k \right) \hat{U}_j - \sum_{\text{initial}} n_i \hat{U}_i + \sum_{\text{rxns}} \xi_k (\Delta \hat{U}_r^\circ)_k = Q$$

Or implicitly accounting for the change in number of moles

$$\sum_{\text{final}} n_j \hat{U}_j - \sum_{\text{initial}} n_i \hat{U}_i + \sum_{\text{rxns}} \xi_k (\Delta \hat{U}_r^\circ)_k = Q$$

Remember: All of these absolute enthalpies imply reference enthalpies at some standard temperature pressure and state of aggregation.

If enthalpy depends only on temperature:

$$\sum_{\text{out streams}} \dot{n}_j \int_{T_{\text{ref}}}^{T_{\text{out}}} C_{pj} dT - \sum_{\text{in streams}} \dot{n}_i \int_{T_{\text{ref}}}^{T_{\text{in}}} C_{pi} dT + \sum_{\text{rxns}} \dot{\xi}_k (\Delta \hat{H}_r^\circ)_k = \dot{Q}$$

$$\text{where } \dot{n}_j = \dot{n}_i + \sum_{\text{rxns}} \nu_{ik} \dot{\xi}_k.$$

The second method is to choose as reference states the pure *elements* at standard temperature and pressure. The enthalpy of a given species is then the *enthalpy of formation* plus any changes due to temperature ($\int C_p dT$), pressure, solution, or such. The first law then becomes:

$$\sum_{\text{out streams}} \dot{n}_j \hat{H}_j - \sum_{\text{in streams}} \dot{n}_i \hat{H}_i = \dot{Q}$$

and its variants.

Don't forget about latent heats and enthalpies of solution or mixing