Week 12: Lecture 1

Conservation of Energy for Reacting Systems

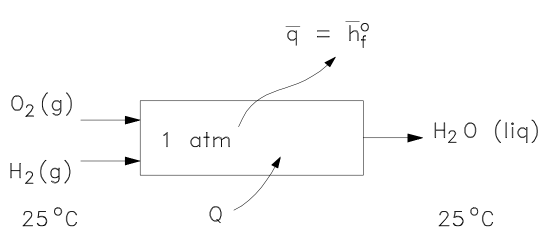
Enthalpy of Formation

- previous calculations involving enthalpy were all based on differences and the reference used to determine enthalpy did not matter
- when chemical reactions occur, reactants disappear and products are formed → differences cannot be calculated for all substances involved
- it is necessary to establish a common base to account for differences in composition
- the enthalpy datum for reacting systems is set to zero at standard temperature and pressure
  - $T_{ref} = 25°C \rightarrow 298\ K$
  - $P_{ref} = 1\ atm$
- $h = 0$ assigned to elements in their most stable form i.e. $O_2, N_2, C, etc.$
- the enthalpy of formation is defined as:
  - the energy released or absorbed when a compound is formed from its stable elements at STP

$$\delta\overline{h}_f^o = \overline{h}_{comp}^o - \sum \overline{n_i}\overline{h}_i^o \quad (kJ/kmole)$$

where
$\overline{n}_i$ = # of moles of i'th elemental substance in forming a single mole of compound (unitless)

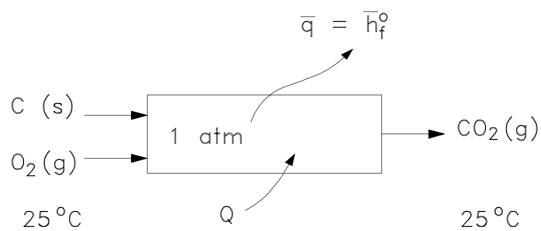
Consider the following reactions taking place at atmospheric pressure, such that $T_{prod} = T_{react} = 298\ K$



$$\frac{1}{2}O_2 + H_2 \rightarrow H_2O$$

where $\overline{h}_f^o = -286\ MJ/kmole\ of\, H_2O$ (heat transferred from the combustion chamber)

Week 12: Lecture 1



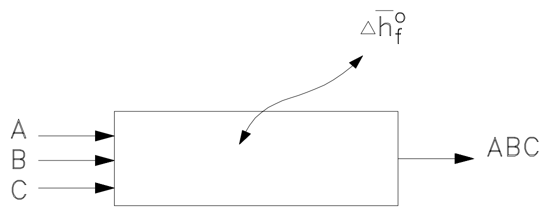
$$C + O_2 \rightarrow CO_2$$

where $\overline{h}_f^o = -393\ MJ/kmole\ of CO_2$ (heat transferred from the combustion chamber)

These reactions are called formation reactions because a substance is formed from its elements in their respective natural states at STP

$$\overline{q} = standard\ heats\ of\ formation$$

$$\overline{h}_f^o = enthalpy\ of\ formation$$



$$\delta\overline{h}_f^o = \overline{h}_{comp}^o - \sum \overline{n}_i \overline{h}_i^o \quad (kJ/kmole)$$

An energy balance gives

$$\underbrace{a\overline{h}_A^o + b\overline{h}_B^o + c\overline{h}_C^o}_{generally\ 0} + \delta\overline{h}_f^o \rightarrow \overline{h}_{ABC}^o$$

If

$\overline{h}_f^o > 0$ - endothermic
$\overline{h}_f^o < 0$ - exothermic