Recap

Task: Determine $\begin{cases} T_O \\ \text{Products' composition } (x_i\text{'s}) \end{cases}$

Treat mixture as ideal gas

Dalton's law

$T_m = T_1 = T_2 \ldots$

$P_m = P_1 + P_2 + \ldots + P_n$

$$\frac{P_i}{P_m} = x_i$$

$$\bar{M}_m = \sum_{i=1}^{n} x_i \bar{M}_i$$

$$\bar{C}_{v_m} = \sum_{i=1}^{n} x_i \bar{C}_{v_i} \quad \text{per mole}$$

$$C_{v_m} = \sum_{i=1}^{n} m_{f_i} C_{v_i} \quad \text{per mass}$$

$$\gamma_m = \frac{C_{pm}}{C_{vm}} = \frac{\bar{C}_{pm}}{\bar{C}_{vm}}$$

Thermodynamics of combustion

In combustion, chemical bonds of a compound (e.g. CH_4) or molecular element (e.g. H_2) are broken and new chemical bonds are formed (e.g. CO_2, H_2O) and the difference in chemical bond energy is released in the form of "sensible heat"

To account for this, use "absolute enthalpy"

@ ref. Temp & pres.

$$h(T) = h_f^o(T_{ref}) + \underbrace{\Delta h_s}_{\Delta h \text{ to go from } T_{ref} \text{ to } T} \qquad (\text{per mass})$$

h of formation

OR

$$\bar{h}(T) = \bar{h}_f^o(T_{ref}) + \Delta\bar{h}_s \qquad (\text{per mole})$$

In our book, $\bar{h}_f^o = Q_f$

Examples of Q_f are in table 2.1

Ex. of exothermic reaction
$\underbrace{\text{exothermic}}_{\text{heat released}}$

$C + O_2 \longrightarrow CO_2 \quad -393.5 \frac{kJ}{mol}$

released → need to remove this heat s.t. $T(CO_2) = T(C+O_2)$

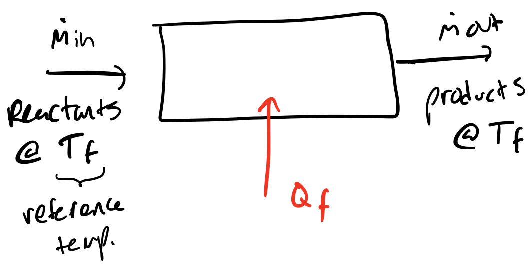
$H_2 + \frac{1}{2}O_2 \longrightarrow H_2O - 241.8 \frac{kJ}{mol}$

Ex. of endothermic:

$O_2 \longrightarrow 2O + 2 \cdot 249.2 \; kJ/mol$

supply

Schematically



- Steady state nrg eq:

$H_{out} - H_{in} = Q$ (No mech. work exchanged)

$Q > 0$ if supplied to system

Here: $H_{products} - H_{reactants} = Q_f$

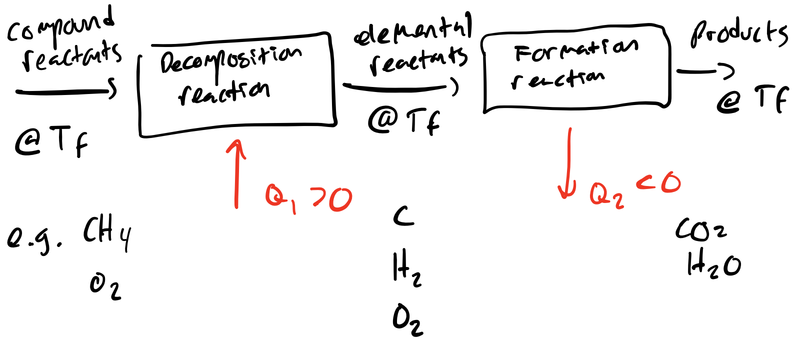
In exothermic rxn, for $T_{in} = T_{out} = T_f = \text{const}$

$Q_f < 0$ (released by rxn)

to keep $T_{in} = T_{out}$, must remove the heat released $(Q_f < 0)$

For a reaction starting w/ naturally occurring reactants (e.g. O_2, H_2), that schematic is adequate, since $Q_{f\,H_2} = Q_{f\,O_2} = 0$

If rxn between non-naturally occurring reactants, need more complicated, idealized schematic



Must first break bonds in CH_4
to deliver C & H_2
from 1st law: Q_1 must be equal & opposite to the heat of formation
(Q_f) of compound reactants entering decomposition reaction

$$Q_1 = \sum_{i=1}^{\text{reactants}} n_i (-Q_{f_i})_{\text{reactants}}$$

And since these $Q_{f_i} < 0$,
$Q_1 > 0$ (supply)

$$Q_2 = \sum_{j=1}^{\text{products}} n_j (Q_{f_j})_{\text{products}}$$

then for entire rxn : $Q = Q_R = Q_1 + Q_2$

$$= \sum_j (n_j Q_{f_j})_{\text{products}} - \sum_i (n_i Q_{f_i})_{\text{reactants}}$$

Then from $H_{out} - H_{in} = Q$

$$H_{P_f} - H_{R_f} = \sum_j (n_j Q_{f_j})_P - \sum_i (n_i Q_{f_i})_R$$

enthalpy of products @ T_f

$H_{P_f} - H_{R_f} \equiv H_{PR_f} \equiv$ enthalpy of combustion