Recap

$$aH_2 + bO_2 \rightarrow cH_2O + dO_2 + eH_2 + fO + gH + hOH$$

Mass bal.
$$\begin{cases} 2a = 2c + 2e + g + h \\ 2b = c + 2d + f + h \end{cases}$$

Equil.
$$\begin{cases} K_{p_1} P_m^{-1} = \dfrac{e^2 d}{c^2 (c + d + e + f + g + h)} \\ \vdots \qquad \cdots \end{cases}$$

① → Kps in plots

② Solve system of nonlinear algebraic eqns ①-⑥

③

④

⑤

⑥ If T, P_m known → Find c, d, e, ... = product composition

If T, P_m unknown,

Pick P_m
  Pick T
    solve eq. 1-6
  Loop
Loop

For H_2O, simplified reactions are in fig. 2.13

More complex rxn in fig. 2.14

Remarks

- low temperature → less dissociation (more H_2O)
- In simplified system (fig. 2.13) high P → less dissociation
- In more complicated sys. (fig. 2.14)

  H_2, O_2, OH curves not monotonic

  @ Low T & high P → lower H_2, O_2, OH concentration

  @ High T & high P → higher H_2, O_2, OH concentration

Summary

If composition of products is known find T from thermo

If T is known, find composition from chem. equil.

What if neither comp. or T is known?

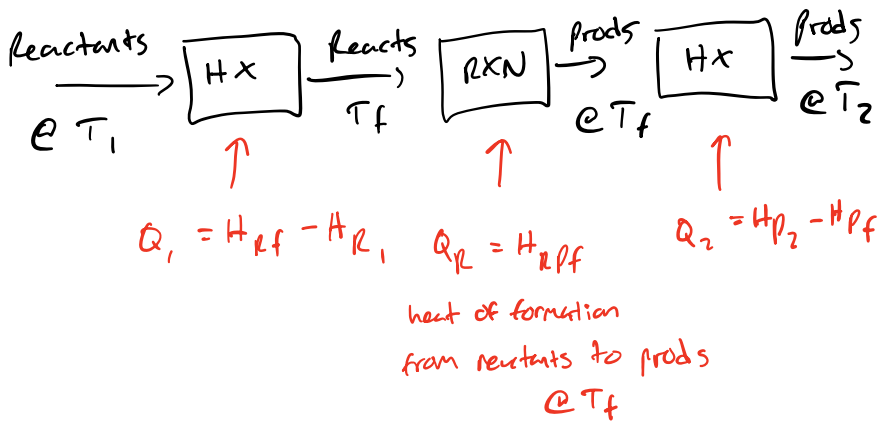
How do we determine both?

Flame temperature

How much heat is released in

$$a H_2 + b O_2 \rightarrow c H_2O + d O_2 + e H_2 + f O + g H + h OH \; ?$$

Recall simple model



For simplicity, assume $T_1 = T_f$, $\rightarrow Q_1 = 0$

$$H_{Rf} = \sum_j (n_j \bar{h}_{f_j})_{prods} - \sum_i (n_i \bar{h}_{f_i})_{reacts}$$

$$Q_2 = H_{P_2} - H_{Rf} = \sum_j n_j (\bar{h} - \bar{h}_o)_{prods}$$

$\bar{h}$ = enthalpy / mole

$\bar{h}_{f_j}$ ← enthalpy @ T_f

$\bar{h}$ ← enthalpy @ T_2 ($=T$)

In this class $\bar{h}(T) = \bar{c}_p T$

more rigorously,

$$\bar{h}(T) = \int_{0K}^{T} \bar{c}_p(T)\, dT$$

Net heat exchanged between sys. & surr

$$Q = \cancel{Q_1}^{\,0} + Q_R + Q_2$$

If $Q > 0$, supplied to sys

$Q < 0$, removed from sys.

From fig. 2.14, for each T, P pair, have all x_j's (i.e. n_j's)

Can plot Q vs. T w/ P as parameter

Results in fig. 2.15

Remarks

@ Low T, $Q < 0$: Even after products reach $T = 3000K$ ($P = 1atm$) Heat is released to outside

@ High T, $Q > 0$: Even after combustion, for products to reach 4000K (at $P_1 = 1atm$), must supply heat

- @ Low P, High dissociation requires more heat to reach a high temperature

- Line through Q = 0 intersects the Q-lines (parameterized by P) @ values of T called "adiabatic flame temperature"

  → corresponds to T_2 in schematic provided system is insulated

Revisit example to compare complete (w/o dissoc.) vs. incomplete (w/ dissoc.) combustion

Recall figs 2.13 (simplified) & 2.14 (more complete model)

$$Q = \underbrace{H_{Rf} - H_{R_1}}_{Q_1} + \underbrace{H_{RPf}}_{Q_R} + \underbrace{(H_{P_2} - H_{Pf})}_{Q_2}$$