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Problem 5.4

Given: $2H_2 + O_2 \rightarrow aH_2O + bO_2 + cH_2 + dOH$
And dissociation reactions
$H_2 + \frac{1}{2}O_2 \leftrightharpoons H_2O$ and $\frac{1}{2}O_2 + \frac{1}{2}H_2 \leftrightharpoons OH$

Find: Balanced chemical equation, molecular weight, characteristic velocity, and specific heat ratio, and adiabatic flame temp

Assumptions: Reactants are at 298K & P = 50 atm
Include temp dependent C_p data from T5.3
Using Purdue's K_p table

Basic Equations:

$$H = h^o + \int c_p \, dT$$

$$\gamma = \frac{c_p}{c_p - R_u}$$

$$c^* = \sqrt{\frac{R_u T_c}{\gamma \mu}}$$

Analysis:

$$2H_2 + O_2 \rightarrow aH_2O + bO_2 + cH_2 + dOH$$

H: $4 = 2a + 2c + d$

O: $2 = a + 2b + d$

$d = 2 - a - 2b$

Sub into H's

$4 = 2a + 2c + 2 - a - 2b$

$2c = 2 - a + 2b$

$c = 1 - \frac{1}{2}a + b$

Rewrite chemical eq

$$2H_2 + O_2 \rightarrow aH_2O + bO_2 + (1 - \tfrac{1}{2}a + b)H_2 + (2 - a - 2b)OH$$

So, the total number of moles is

$n = a + b + 1 - \frac{1}{2}a + b + 2 - a - 2b$

$n = -\frac{1}{2}a + 3$

We also have

$$K_{p,3} = \frac{\chi_{OH}}{\sqrt{\chi_{O_2}\chi_{H_2}}} P^{(1-\frac{1}{2}-\frac{1}{2})}$$

$$K_{p,4} = \frac{\chi_{H_2O}}{\chi_{H_2}\sqrt{\chi_{O_2}}} P^{(1-1-\frac{1}{2})}$$

$$\chi_{H_2O} = \frac{a}{-\frac{1}{2}a+3}, \quad \chi_{H_2} = \frac{1-\frac{1}{2}a+b}{-\frac{1}{2}a+3}, \quad \chi_{O_2} = \frac{b}{-\frac{1}{2}a+3}, \quad \chi_{OH} = \frac{2-a-2b}{-\frac{1}{2}a+3}$$

$$K_{p3} = \frac{\frac{2-a-2b}{-\frac{1}{2}a+3}}{\left(\frac{b}{-\frac{1}{2}a+3}\right)^{1/2}\left(\frac{1-\frac{1}{2}a+b}{-\frac{1}{2}a+3}\right)^{1/2}} = \frac{2-a-2b}{(b+b^2-\frac{1}{2}ab)^{1/2}}$$

$$K_{p4} = \frac{\frac{a}{-\frac{1}{2}a+3}}{\left(\frac{1-\frac{1}{2}a+b}{-\frac{1}{2}a+3}\right)\left(\frac{b}{-\frac{1}{2}a+3}\right)^{1/2}} P^{-1/2} = \frac{a(-\frac{1}{2}a+3)^{1/2}}{b^{1/2}(1-\frac{1}{2}a+b)} P^{-1/2}$$

Reactants = 0 since $h^\circ = 0$ for both H_2 & O_2 and they are injected at 298K

Products:

$$0 = a\left[-57800\,\tfrac{cal}{mol}(4.184)\tfrac{J}{cal} + \int_{298}^{T_c} C_p\,dT\right]_{H_2O} + b\left[\int_{298}^{T_c} C_p\,dT\right]_{O_2}$$

$$+ (1-\tfrac{1}{2}a+b)\left[\int_{298}^{T_c} C_p\,dT\right]_{H_2} + (2-a-2b)\left[10060\,\tfrac{cal}{mol}(4.184)\tfrac{J}{cal} + \int_{298}^{T_c} C_p\,dT\right]_{OH}$$

$$\left.\begin{aligned}
Cp_{H_2O} &= 29.182 + 14.503\,(T/1000) - 2.0235\,(T/1000)^2 \\
Cp_{O_2} &= 28.186 + 6.3011\,(T/1000) - 0.74986\,(T/1000)^2 \\
Cp_{H_2} &= 26.896 + 4.3501\,(T/1000) - 0.32674\,(T/1000)^2 \\
Cp_{OH} &= 81.55 - 15\,(T)^{1/4} + 0.313\,(T)^{3/4} - 0.02\,(T)
\end{aligned}\right\}\ \frac{J}{gmol\,K}$$

Plug these in to enthalpy balance, guess T_c, check K_p, get a & b, determine $H_1 = H_2$. Iterate & repeat

For P = 50 atm,

$$\boxed{\begin{aligned} &T_c = 3584.517\ K \\ &a = 1.471,\ b = 0.115,\ c = 0.379,\ d = 0.299 \end{aligned}}$$

$$\boxed{2H_2 + O_2 \rightarrow 1.471\ H_2O + 0.115\ O_2 + 0.379\ H_2 + 0.299\ OH}$$

$$M = \frac{1.471}{-\tfrac{1}{2}(1.471)+3}(18) + \frac{0.115}{-\tfrac{1}{2}(1.471)+3}(32) + \frac{0.379}{\tfrac{1}{2}(1.471)+3}(2) + \frac{0.299}{\tfrac{1}{2}(1.471)+3}(17)$$

$$\boxed{M = 15.898\ g/gmol}$$

Specific heat ratio

$$\gamma = \frac{Cp}{Cp - R_u} \qquad Cp \text{ total (excel)} = 142.517\ J/gmol\,K$$

$$\gamma = \frac{142.5}{142.5 - 8.317}$$

$$\boxed{\gamma = 1.06195}$$

Char vel

$$C^* = \sqrt{\frac{R_u T_c}{\gamma M}} = \sqrt{\frac{8.314\ \tfrac{Nm}{gmol\,K} \times 3584.5K \times 1000g/kg}{1.06195 \times 15.898\ g/gmol}}$$

$$\boxed{C^* = 1328.6\ m/s}$$