Assignment - 4 AE330

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Ans 1) Given $\phi = 1$ $\Rightarrow$ Stiochiometric equation,

$T_1 = 298$

$\Delta H^\circ_{H_2O} = -241.997$ kJ/mol,

C_p of H_2O = 53.9 kJ/kmol

Reaction

↳ $2H_2 + O_2 \rightarrow 2H_2O$ [Stiochiometric reaction]

Now, we can say that,

$$\Delta H_{reactants} = \Delta H_{products}.$$

$$\Delta H_{reactants} = 2\Delta H^\circ_{H_2} + \Delta H^\circ_{O_2} + 2C_{pH_2}(T_1 - T_{ref}) + C_{pO_2}(T_1 - T_{ref})$$

As H_2, O_2 are naturally occuring,

$\Delta H^\circ_{H_2}$, $\Delta H^\circ_{O_2} = 0$ & $T_1 = T_{ref} = 298$ K,

$$\Delta H_{reactants} = 0.$$

$$\Delta H_{products} = 2 \cdot \Delta H^\circ_{H_2O} + 2 \cdot C_{p\,H_2O}(T_{ad} - 298)$$

$$\Delta H_{products} = 2 \cdot (-241.997) + 2 \cdot 0.0539 (T_{ad} - 298)$$

As $\Delta H_{reactant} = \Delta H_{products}$

$$\Rightarrow \quad T_{ad} = 298 + \frac{\times 241.997}{0.0539}$$

$$\boxed{T_{ad} = 4787.74 \text{ K}}$$

[Adiabatic Flame Temperature]

Ans 2) This is a more realistic case of question 1.

$$2H_2 + O_2 \rightarrow 1.83H_2O + 0.17H_2 + 0.085O_2$$

As we found in question 1, $\Delta H_{reactants} = 0$ at $T_1 = 298$ K.

For $\Delta H_{products}$,

Species	n	$\Delta H^o_{formation}$	$C_{pi}(T_{ad} - T_{ref})$
H_2O	1.83	$-\cancel{29}241.997$	$0.0539\,(T_{ad} - 298)$
H_2	0.17	0	$0.0358\,(T_{ad} - 298)$
O_2	0.085	0	$0.0389\,(T_{ad} - 298)$

As $\Delta H_{reactants} = \Delta H_{product}$

$$0 = (1.83)(-241.997) + (1.83)(0.0539)(T_{ad} - 298) + (0.17)(0.0358)(T_{ad} - 298) + (0.085)(0.0389)(T_{ad} - 298)$$

$$442.8545 = 0.10803\,(T_{ad} - 298)$$

$$\boxed{T_{ad} = 4397.385 \text{ K}}$$

As we can see, if we consider equilibrium effects the T_{ad} is less than the ideal case by around 385 K

For average molecular mass,

$$MW_{avg} = \sum_{products} X_i (MW)_i$$

$X_i \rightarrow$ Mole fraction

$MW_i \rightarrow$ Mol mass of the species.

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$$(MW_{avg}) = \frac{1.83}{2.085} \times 18 + \frac{0.17}{2.085} \times 2 + \frac{0.085}{2.085} \times 32$$

$$\boxed{MW_{avg} = 17.266 \text{ g}}$$

$$R_p = \frac{R_u}{MW_{avg}} = \frac{8.314}{0.017266} = \boxed{481.524 \text{ J/Kg-K}}$$

Now, $C_p - C_v = R_u$, But for that we need to find $C_{p(avg)}$ for the products

$$C_{p(avg)} = \sum X_i C_{pi} \quad (\text{In kJ/kmol-K})$$

$$= \frac{1.83}{2.085} \times 53.9 + \frac{0.17}{2.085} \times 35.811 + \frac{0.085}{2.085} \times 38.9$$

$$= 47.31 + 2.9198 + 1.6328$$

$$\boxed{C_{p(avg)} = 51.862 \text{ kJ/Kmol-K}}$$

Now, $C_{v(avg)} = C_{p(avg)} - R_u$

$$C_{v(avg)} = 43.548 \text{ kJ/kmol-k}$$

Now we can find k_{avg} for products,

$$k = \frac{C_p}{C_v} \Rightarrow \boxed{k_{avg} = 1.191}$$, Hence,

$$C^* = \frac{\sqrt{kRT_{ad}}}{k\sqrt{\left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}}} \Rightarrow \boxed{C^* = 2.25 \text{ km/sec}}$$

Ans 3) Given, Fuel ⇒ Kerosene, ($C_{12}H_{24}$)

$\phi = 1$ ⇒ Stiochometric Equation.

$T_1 = 298\,K = T_{ref}$.

⇒ Reaction can be written as,

$$C_{12}H_{24} + 18\,O_2 \longrightarrow 12CO_2 + 12H_2O$$

For ΔH_r we can write,

$$\Delta H_r = 1 \times \left[\Delta H^\circ_{kerosene} + C_{p,kerosene}(T_1 - T_{ref})\right]$$
$$18 \times \left[\Delta H^\circ_{O_2} + C_{p,O_2}(T_1 - T_{ref})\right]$$

$$\boxed{\Delta H_r = -159\ kJ/mol}$$

For ΔH_p,

$$\Delta H_p = 12\left[\Delta H^\circ_{CO_2} + C_{p,CO_2}(T_{ad} - T_{ref})\right]$$
$$+ 12\left[\Delta H^\circ_{H_2O} + C_{p,H_2O}(T_{ad} - T_{ref})\right] = H_R$$

$$\frac{-159}{12} = -393.978 + 0.06043(T_{ad} - \cancel{T_R}\,298)$$
$$-241.997 + 0.0539\,(T_{ad} - 298)$$

$$(0.11433)(T_{ad} - 298) = \cancel{622.225}\ 622.725$$

$$T_{ad} = 298 + \frac{622.725}{0.11433}$$

$$\boxed{T_{ad} = 5744.73\ K}$$

Stiochiometric mixture ratio can be found as,

$C_{12}H_{24} + 18O_2 \rightarrow$ Products at $\phi = 1$.

$$(MR)_{st} = \frac{(18)\,32}{168}$$

$$\boxed{\Rightarrow (MR)_{st} = 3.4286}$$

Ans 4) Now instead of the Stoichiometric combustion, we have, $\phi = 1.2$ (Fuel Rich) (Incomplete combustion)

But as in this case, we don't have information about carbon monoxides, we will assume that methane either gets converted to CO_2, or doesn't get reacted at all.

The stiochiometric reaction of Methane combustion is,

$$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2$$

from this we can find, $(MR)_{st}$ as,

$$(MR)_{st} = \frac{2\,(32)}{16} = 4$$

Given, $\phi = \frac{(MR)_{st}}{MR} = 1.2 \Rightarrow \boxed{MR = 10/3}$

Let the current reaction require 'n' moles of O_2 for 1 mole of CH_4,

$$MR = \frac{(n)\,32}{16} = 10/3 \Rightarrow n = 5/3$$

Hence we can now write the reaction as,

$$CH_4 + \frac{5}{3}(O_2 + 3.76N_2) \longrightarrow \frac{5}{6}CO_2 + \frac{5}{3}H_2O + \frac{1}{6}CH_4 \text{ (unreacted)}$$
$$+ 6.267N_2$$

Now given the values of $\Delta h^{\circ}_{f_i}$ & C_{p_i}, we can write

$$\Delta H_R = 1 \times \left(\Delta h^\circ_{f,CH_4} + (T_1 - T_{ref})\, C_{p,CH_4}\right)$$

$$+ \frac{5}{3} \times \left(\Delta h^\circ_{f,O_2} + C_{p,O_2}(T_1 - T_{ref})\right)$$

$$+ \frac{5}{3}(3.76)\left(\Delta h^\circ_{f,N_2} + C_{p,N_2}(T_1 - T_{ref})\right)$$

Now assuming $T_1 = T_{ref} = 298K$ for simplicity,

$$\boxed{\Delta H_R = -74.83}$$

Now, for ΔH_P

$$\Delta H_P = \frac{5}{6}\left(\Delta h^\circ_{f,CO_2} + C_{p,CO_2}(T_{ad} - T_{ref})\right)$$

$$+ \frac{5}{3}\left(\Delta h^\circ_{f,H_2O} + C_{p,H_2O}(T_{ad} - T_{ref})\right)$$

$$+ \frac{1}{6}\left(\Delta h^\circ_{f,CH_4} + C_{p,CH_4}(T_{ad} - T_{ref})\right)$$

$$+ 6.267\left(\Delta h^\circ_{f,N_2} + C_{p,N_2}(T_{ad} - T_{ref})\right)$$

$$\Delta H_p = \frac{5}{6}(-393.978) + \frac{5}{3}(-241.997) + \frac{1}{6}(-74.83) + 6.267 \times 0$$

$$+ \left[\frac{5}{6}(0.0562) + \frac{5}{3}(0.0439) + \frac{1}{6}(0.0358) + 6.267(0.0337)\right](T_{ad} - 298)$$

Equating ΔH_R & ΔH_p, we get

$$-74.83 = -744.115 + 0.3371(T_{ad} - 298)$$

$$\Rightarrow \boxed{T_{ad} = 2283.42\ K}$$

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