HW4 p2

2020年2月9日 日曜日　　午後2:31

Problem 2. Heat of reaction and adiabatic flame temperature of a simple reaction

Propane ($\Delta h_f^0 = -104\ kJ/mole$) and air react at 298K and 1 atm and at $\phi = 0.8$. Remember to start by writing the chemical equation for this reaction at $\phi = 1.0$, and then adjust the reaction to the given equivalence ratio. Assume the product stream comprises only H_2O, CO_2, and what is left over from the excess reactants. Calculate the heat of reaction, in terms of kJ/mole of propane. Then calculate the adiabatic flame temperature at $\phi = 0.8$. Consider the temperature dependency of heat capacity in your calculation by using the table of $c_p(T)$ in Appendix II of your textbook. To balance the heat of reaction with the temperature rise of the products, $-\Delta H_{rxn} = \sum_{products,i} \int_{T^0}^{T_{ad}} n_i c_{p,i} dT$, use one of two methods. The first uses an iterative approach - guess a value for the AFT, and then check the energy balance by calculating the right hand side term. Iterate until successive estimates of the temperatures converge within 150K. Alternatively, construct a table of the RHS term as a function of T, and determine T_{ad} by inspection of the table. Next, use CEA (https://cearun.grc.nasa.gov/) to calculate the flame temperature and compare it to your final estimate. Compare the composition of the combustion products from CEA and your written chemical reaction at $\phi = 0.8$ in terms of their mole fractions.

(i) Chemical eqn.

propane C_3H_8 : $CH_3-CH_2-CH_3$ $\quad M_{C_3H_8} = 44\ g/mol$

the balanced chemical rxn becomes (air N_2 : 79% O_2 : 21%)

$\because\ 5 \div 21 \times 79 = 18.81$

$$\boxed{C_3H_8(g) + 5\,O_2(g) + 18.81\,N_2(g) = 3\,CO_2(g) + 4\,H_2O(g) + 18.81\,N_2(g)}$$

stoichiometric

now since $\varphi = 0.8$

we know that $\frac{1}{0.8} = 1.25$ times more O_2 exists than wrt stoichiometric conditions

$5 \times 1.25 = 6.25$, $18.81 \times 1.25 = 23.513$

than the balanced rxn equation becomes

$$\boxed{C_3H_8(g) + 6.25\,O_2(g) + 23.513\,N_2(g) = 3CO_2(g) + 4H_2O(g) + 23.513N_2(g) + 1.25\,O_2(g)}$$

(ii) heat of rxn.

the heat of formation for each reactants & products are from the lecture slide

C_3H_8: -103.8 kJ/mol From: https://webbook.nist.gov/cgi/cbook.cgi?ID=C74986&Mask=1

N_2 : 0

O_2 : 0

CO_2 : -393.522 kJ/mol

H_2O : -241.826 kJ/mol

$$\therefore \Delta H^\circ = [3\times(-393.522\ \text{kJ/mol}) + 4\times(-241.826\ \text{kJ/mol})] - [-103.8\ \text{kJ/mol}]$$

$$= \boxed{-2044.07\ \text{kJ/mol propane}}$$

(iii) adiabatic temperature

since C_p is a func of θ (on the slides)

N_2: $C_{p0} = 39.060 - 512.79\,\theta^{-1.5} + 1072.7\,\theta^{-2} - 820.40\,\theta^{-3}$

O_2: $C_{p0} = 37.432 + 0.020102\,\theta^{1.5} - 178.57\,\theta^{-1.5} + 236.88\,\theta^{-2}$

$$
\begin{cases}
N_2: \ \bar{C}_{p0} = 39.060 - 512.79\theta^{-1.5} + 1072.7\theta^{-2} - 820.40\theta^{-3} \\
O_2: \ \bar{C}_{p0} = 37.432 + 0.020102\theta^{1.5} - 178.57\theta^{-1.5} + 236.88\theta^{-2} \\
CO_2: \ \bar{C}_{p0} = -3.7357 + 30.529\theta^{0.5} - 4.1034\theta + 0.024198\theta^{2} \\
H_2O: \ \bar{C}_{p0} = 143.05 - 183.54\theta^{0.25} + 82.751\theta^{0.5} - 3.6989\theta
\end{cases}
$$

now from

$$
-\Delta H_{rxn} = \sum_{products,i} \int_{T_{ref}}^{T_{ad}} n_i C_{p,i}\, dT
$$

$$
\begin{cases}
\theta = \frac{T}{100} \iff d\theta = \frac{dT}{100} \iff dT = 100\, d\theta \\
T: T_{ref} \to T_{ad} \iff \theta: \frac{T_{ref}}{100} = \theta_{ref} \to \frac{T_{ad}}{100} = \theta_{ad}
\end{cases}
$$

$$
-(-2044.07 \ kJ/mol) = \sum_{product,i} \int_{\theta_{ref}}^{\theta_{ad}} 100\, n_i C_{p,i}\, d\theta \quad \left(\theta : \cancel{kJ/kmol} = J/mol\right)
$$

$$\Downarrow$$

$$
{}^{*}\left(2044.07 \ kJ/mol\right) \cdot \frac{1000\ J}{1\ kJ} = 2{,}044{,}070
$$

(matlab code is in appendix)

solving by using optimization method in MATLAB by minimizing the function below (to zero)

$$
abs\left[\sum_{products,i} \int_{T_{ref}}^{T_{ad}} n_i C_{p,i}\, dT + \Delta H_{rxn}\right]
$$

$$\boxed{T_{ad} = 2052.43\ K}$$

next, using CEA we get

$$\boxed{T_{ad} = 2040.47\,K}$$

(CEA results are in the appendix)

the error is

$$\boxed{\text{error} = 11.96\,K}$$

the mole fractions for my & CEAs analyses

my		CEA	
N_2:	0.74026	N_2:	0.72918
O_2:	0.03935	O_2:	0.03746
CO_2:	0.09445	CO_2:	0.09354
H_2O:	0.12593	H_2O:	0.12422

for all product elements they are close to identical with approximately 1% difference.