

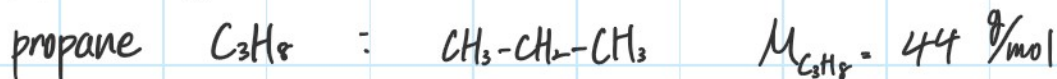
HW4 p2

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

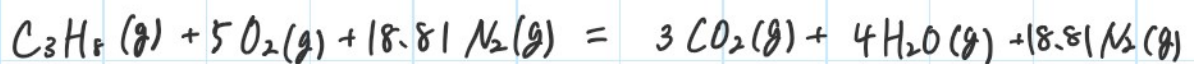
Propane ($\Delta h_f^0 = -104 \text{ kJ/mole}$) and air react at 298K and 1 atm and at $\phi = 0.8$. Remember to start by writing the chemical equation for this reaction at $\phi = 1.0$, and then adjust the reaction to the given equivalence ratio. Assume the product stream comprises only H_2O , CO_2 , 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.



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

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



now since $\phi = 0.8$

stoichiometric

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

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

then the balanced rxn equation becomes



(ii) heat of rxn.

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

$$\text{C}_3\text{H}_8: -103.8 \text{ kJ/mol}$$

From: <https://webbook.nist.gov/cgi/cbook.cgi?ID=C74986&Mask=1>

$$\text{N}_2: 0$$

$$\text{O}_2: 0$$

$$\text{CO}_2: -393.522 \text{ kJ/mol}$$

$$\text{H}_2\text{O}: -241.826 \text{ kJ/mol}$$

$$\begin{aligned} \therefore \Delta H^\circ &= [3 \times (-393.522 \text{ kJ/mol}) + 4 \times (-241.826 \text{ kJ/mol})] - [-103.8 \text{ kJ/mol}] \\ &= -2044.07 \text{ kJ/mol} \quad \text{propane} \end{aligned}$$

(iii) adiabatic temperature

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

$$\begin{aligned} \int \text{N}_2: \bar{C}_{p0} &= 39.060 - 512.79\theta^{-1.5} + 1072.70\theta^{-2} - 820.40\theta^{-3} \\ \int \text{O}_2: \bar{C}_{p0} &= 37.432 + 0.020102\theta^{1.5} - 178.57\theta^{-1.5} + 236.88\theta^{-2} \end{aligned}$$

$$\left\{ \begin{array}{l} N_2: \bar{C}_{p0} = 39.060 - 512.79\theta^{-1.5} + 1072.7\theta^{-4} - 820.40\theta^{-3} \\ O_2: \bar{C}_{p0} = 37.432 + 0.020102\theta^{1.5} - 178.57\theta^{-1.5} + 236.88\theta^{-2} \\ CO_2: \bar{C}_{p0} = -3.7357 + 30.529\theta^{0.5} - 4.1034\theta + 0.024198\theta^2 \\ H_2O: \bar{C}_{p0} = 143.05 - 183.54\theta^{0.25} + 82.751\theta^{0.5} - 3.6989\theta \end{array} \right.$$

now from

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

$$\left\{ \begin{array}{l} \theta = \frac{T}{100} \Leftrightarrow d\theta = \frac{dT}{100} \Leftrightarrow dT = 100 d\theta \end{array} \right.$$

$$\left\{ \begin{array}{l} T: T_{ref} \rightarrow T_{ad} \Leftrightarrow \theta: \frac{T_{ref}}{100} = \theta_{ref} \rightarrow \frac{T_{ad}}{100} = \theta_{ad} \end{array} \right.$$

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

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

(matlab code is in appendix)

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

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

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

next, using CEA we get

$$T_{ad} = 2040.47 \text{ K}$$

(CEA results are in the appendix)

the error is

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

the mole fractions for my & CEA's analyses

my

N_2 : 0.74026

O_2 : 0.03935

CO_2 : 0.09445

H_2O : 0.12593

CEA

N_2 : 0.72918

O_2 : 0.03946

CO_2 : 0.09354

H_2O : 0.12422

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