ME 354 Tutorial, Week#13
Reacting Mixtures

Question 1:
Determine the mole fractions of the products of combustion when octane, \(C_8H_{18}\), is burned with 200% theoretical air. Also, determine the air-fuel ratio and the dew-point temperature of the products if the pressure is 0.1 MPa.

Step 1: Draw a diagram to represent the system

Step 2: State your assumptions
Assumptions:
1) Combustion is complete
2) Combustion gases are ideal gases
3) Steady operating conditions exist

Step 3: Solve
Before we start the solution to this problem let us examine the general cases of complete combustion to develop a procedure for balancing the reaction equations.

For Excess Air and Complete Combustion

\[
C_8H_{18} + b(1 + a)(O_2 + 3.76N_2) \rightarrow xCO_2 + yH_2O + abO_2 + zN_2
\]

Let \((1+a)\) = the percent of theoretical air, where “a” is the percentage of excess air. [For example, for 300% theoretical air (200% excess air), \((1+a)=3\) so \(a=2\)].

\[
C_8H_{18} + b(2)(O_2 + 3.76N_2) \rightarrow xCO_2 + yH_2O + bO_2 + zN_2
\]

The problem states that octane, \(C_8H_{18}\), is combusted with 200% theoretical air (or 100% excess air) so \(a = 1\). Using the formulas developed for the general case with excess air the stochiometric coefficients can be determined as shown below.
\[ C: \rightarrow 8 = x \]
\[ H: \rightarrow 18 = 2y \quad \text{So, } y = 9 \]
\[ O: \rightarrow 2x \times 2b = 2x + y + 2b \quad \text{So, } b = 12.5 \quad \text{(corrected)} \]
\[ N: \rightarrow 2x \times 3.76x \times b = 2z \quad \text{So, } z = 94 \quad \text{(corrected)} \]

The balanced reaction equation is shown below in Eq1.

\[
C_8H_{18} + 25(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 12.5O_2 + 94N_2 \quad \ldots \ldots \text{Eq 1}
\]

[a] The total moles of products, \( N_{\text{products}} \), can be determined by adding the number of moles of each product as shown below.

\[
\begin{align*}
N_{\text{CO}_2} &= 8 \text{ K mole} \\
N_{\text{H}_2\text{O}} &= 9 \text{ K mole} \\
N_{\text{O}_2} &= 12.5 \text{ K mole} \\
N_{\text{N}_2} &= 94 \text{ K mole}
\end{align*}
\]

\[
N_{\text{products}} = (8 + 9 + 12.5 + 94) = 123.5 \text{ K mole}
\]

The mole fractions, \( y_i \), of each component are determined below:

\[
\begin{align*}
y_{\text{CO}_2} &= \frac{N_{\text{CO}_2}}{N_{\text{products}}} = \frac{8}{123.5} = 6.47\% \\
y_{\text{H}_2\text{O}} &= \frac{N_{\text{H}_2\text{O}}}{N_{\text{products}}} = \frac{9}{123.5} = 7.29\% \\
y_{\text{O}_2} &= \frac{N_{\text{O}_2}}{N_{\text{products}}} = \frac{12.5}{123.5} = 10.12\% \\
Y_{\text{N}_2} &= \frac{N_{\text{N}_2}}{N_{\text{products}}} = \frac{94}{123.5} = 76.12\%
\end{align*}
\]

Answer 1a)

[b] The air-Fuel Ratio, \( AF = \frac{m_{\text{AIR}}}{m_{\text{FUEL}}} \left( \frac{Kg_{\text{AIR}}}{Kg_{\text{FUEL}}} \right) \) \ldots \ldots \text{Eq.-2}

\[
m_{\text{AIR}} = N_{\text{AIR}} \times M_{\text{AIR}}
\]

Where

\[
N_{\text{AIR}} = 25 \times (1 + 3.76) [Kmole] \quad \text{(From Balanced Reaction Equation)}
\]

\[
M_{\text{AIR}} = 29 \left( \frac{Kg_{\text{AIR}}}{Kmole} \right) \quad \text{(From Table A-2 of Text Book)}
\]

Similarly.

\[
m_{\text{FUEL}} = N_{\text{FUEL}} \times M_{\text{FUEL}}
\]

Where

\[
N_{\text{FUEL}} = 1 [Kmole] \quad \text{(From Balanced Reaction Equation)}
\]
From Equation 2, substituting all values, we get,

\[
M_{FUEL} = M_{C_{2}H_{6}} = (8 \times 12.012 + 18 \times 1.008) \left( \frac{Kg_{FUEL}}{Kmole} \right)
\]

So, \( M_{FUEL} = 114.24 \left( \frac{Kg_{FUEL}}{Kmole} \right) \)

From Equation 2, substituting all values, we get,

\[
AF = \frac{m_{AIR}}{m_{FUEL}} = \frac{25 \times (1 + 3.76) [Kmole] \times 29 \left( \frac{Kg_{AIR}}{Kmole} \right)}{1 [Kmole] \times 114.24 \left( \frac{Kg_{FUEL}}{Kmole} \right)}
\]

\[
AF = 30.1 \left( \frac{kg_{AIR}}{kg_{FUEL}} \right)
\]

The dew-point temperature of the products is the temperature at which the water vapor in the products starts to condense as the products are cooled. This is the saturated temperature corresponding to the pressure of \( H_{2}O \) (i.e. the partial pressure of \( H_{2}O \) in the mixture). Since it is assumed that the combustion gases behave as ideal gases, the partial pressure of \( H_{2}O \) can be determined from the total pressure multiplied by the mole fraction of \( H_{2}O \), \( y_{H2O} \).

\[
\rightarrow P_{H2O} = y_{H2O}P = (0.0729)(0.1 \text{ [MPa]}) = 7.29 \text{ kPa}
\]

From Table A-4, interpolating in between 35°C and 40°C

\[
\frac{T_{dp} - 35}{40 - 35} = \frac{7.287 - 5.628}{7.384 - 5.628} \rightarrow T_{dp} = 39.72^\circ C
\]

**Answer 1b)**
**Question 2:**
A small gas turbine uses C₈H₁₈ (l) for fuel, with 400% theoretical air. The air and fuel enter at 25°C and the products of combustion leave at 900K. The output of the engine and the fuel consumption are measured, and it is found that the specific fuel consumption is 0.25 kg/s of fuel per megawatt output. Determine the heat transfer from the engine per kmol of fuel. Assume complete combustion.

**Step 1: Draw a diagram to represent the system**

![Diagram of combustion chamber](image)

**Step 2: State your assumptions**
Assumptions:
1) Combustion is complete
2) Combustion gases are ideal gases
3) Δke, Δpe ≈ 0
4) steady operating conditions exist

**Step 3: Solve**
Using the procedures developed in Question #1, the reaction equation can be balanced for 400% theoretical air (a=3) as shown below.

\[
\begin{align*}
\text{C's} & \rightarrow n_{O_2} = x = 8 \\
\text{H}_2\text{'s} & \rightarrow n_{H_2O} = \frac{y}{2} = \frac{18}{2} = 9 \\
\text{O}_2\text{'s} & \rightarrow n_{O_2} = x + \frac{y}{4} = 8 + \frac{18}{4} = 12.5 \\
\text{N}_2\text{'s} & \rightarrow n_{N_2} = 3.76(1+a)n_{O_2} = 3.76(4)(12.5) = 188
\end{align*}
\]

\[C_8H_{18} + 50(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 37.5O_2 + 188N_2\]

In order to determine the heat transfer from the system a first law analysis can be performed on the combustion chamber. A general first law equation for combustion analysis (on a “per mole of fuel basis”) is shown in Eq1.

\[Q_{in} + W_{in} + \sum N_r(h_f + h - h^\circ)_r = Q_{out} + W_{out} + \sum N_p(h_f + h - h^\circ)_p \quad \text{(Eq1)}\]
The heat transfer and work will be assumed to be out of the system so $Q_{in}$ & $W_{in}$ terms are zero. The enthalpies for the reactants will be determined first. Note: the circle superscript is used to denote that the property value is referenced to a 25°C, 1atm reference state.

**Reactants (C$_8$H$_{18}$, O$_2$, and N$_2$)**

*Enthalpy of formation, $\bar{h}^\circ_f$*

For stable elements O$_2$ and N$_2$, the enthalpy of formation is zero

$\rightarrow \bar{h}^\circ_{f,O_2} = 0$

$\rightarrow \bar{h}^\circ_{f,N_2} = 0$

The enthalpy of formation for C$_8$H$_{18}$ (l), is found in Table A-26

$\rightarrow \bar{h}^\circ_f = -249950 \text{ kJ/kmol}$

*Ideal Gas Enthalpy relative to reference state, $\bar{h} - \bar{h}^\circ$*

In the $\bar{h} - \bar{h}^\circ$ term, the $\bar{h}$ term is the ideal gas enthalpy at the temperature of interest and $\bar{h}^\circ$ is the ideal gas enthalpy at the reference temperature. By subtracting $\bar{h}^\circ$ from $\bar{h}$ the ideal gas enthalpy at the temperature of interest is referenced to an ideal gas enthalpy of zero at the reference state. Doing this for all the reactants and products ensures that all the enthalpy values are referenced to the same reference state (25°C, 1atm) and are thus comparable.

Since the reactants are already at the reference state, $\bar{h} - \bar{h}^\circ = 0$ for all the reactants.

$\rightarrow (\bar{h} - \bar{h}^\circ)_{O_2} = 0$

$\rightarrow (\bar{h} - \bar{h}^\circ)_{N_2} = 0$

$\rightarrow (\bar{h} - \bar{h}^\circ)_{C_8H_{18}} = 0$

**Products (CO$_2$, H$_2$O, O$_2$, and N$_2$)**

*Enthalpy of formation, $\bar{h}^\circ_f$*

For stable elements O$_2$ and N$_2$, the enthalpy of formation is zero

$\rightarrow \bar{h}^\circ_{f,O_2} = 0$

$\rightarrow \bar{h}^\circ_{f,N_2} = 0$
The enthalpy of formations for CO₂ and H₂O(g), and located in Table A-26
\[ \Delta h^*_{\text{CO}_2} = -393520 \text{ kJ/kmol} \]
\[ \Delta h^*_{\text{H}_2\text{O}} = -241820 \text{ kJ/kmol} \]

*Ideal Gas Enthalpy relative to reference state, \( \bar{h} - \bar{h}^* \)*

Since the products are at 900K, \( \bar{h} \) at 900K must first be determined and then \( \bar{h} \) at the reference state of 25°C/298K (this is \( \bar{h}^* \)) must be subtracted to ensure the enthalpies are all calculated with respect to the same reference state.

**For CO₂,**
\[ \bar{h}_{900K} = 37405 \text{ kJ/kmol} \text{ (Table A-20)} \]
\[ \bar{h}^* = \bar{h}_{298K} = 9364 \text{ kJ/kmol} \text{ (Table A-20)} \]
\[ \Delta (\bar{h} - \bar{h}^*)_{\text{CO}_2} = 28041 \text{ kJ/kmol} \]

**For H₂O (g),**
\[ \bar{h}_{900K} = 31828 \text{ kJ/kmol} \text{ (Table A-23)} \]
\[ \bar{h}^* = \bar{h}_{298K} = 9904 \text{ kJ/kmol} \text{ (Table A-23)} \]
\[ \Delta (\bar{h} - \bar{h}^*)_{\text{H}_2\text{O}} = 21924 \text{ kJ/kmol} \]

**For O₂,**
\[ \bar{h}_{900K} = 27928 \text{ kJ/kmol} \text{ (Table A-19)} \]
\[ \bar{h}^* = \bar{h}_{298K} = 8682 \text{ kJ/kmol} \text{ (Table A-19)} \]
\[ \Delta (\bar{h} - \bar{h}^*)_{\text{O}_2} = 19246 \text{ kJ/kmol} \]

**For N₂,**
\[ \bar{h}_{900K} = 26890 \text{ kJ/kmol} \text{ (Table A-18)} \]
\[ \bar{h}^* = \bar{h}_{298K} = 8669 \text{ kJ/kmol} \text{ (Table A-18)} \]
\[ \Delta (\bar{h} - \bar{h}^*)_{\text{N}_2} = 18221 \text{ kJ/kmol} \]

The specific fuel consumption is given as 0.25 kg/s of fuel per megawatt output of the engine. This information can be used to find \( W_{\text{out}} \) as shown below.
Note: The molar mass of C\textsubscript{8}H\textsubscript{18} was determined from the molar mass of C (12.012kg/kmol) and H (1.008kg/kmol)

\[ M_{\text{fuel}} = 8(12.012) + 18(1.008) = 114.24\text{kg}_{\text{fuel}}/\text{kmol}. \]

Eq1 can be rearranged to isolate for \( Q_{\text{out}} \) as shown in Eq2.

\[ Q_{\text{out}} = \sum N_{r}(\bar{h}_{f}^{\circ} + \Delta \bar{h}) \cdot W_{\text{out}} - \sum N_{p}(\bar{h}_{f}^{\circ} + \Delta \bar{h})_{p} \quad (\text{Eq2}) \]

Substituting in the values determined above into Eq2 the heat transfer from the engine is determined. Note: the number of moles of each product are determined using the balanced reaction equation: \( N_{\text{CO2}} = 8 \), \( N_{\text{H2O}} = 9 \), \( N_{\text{O2}} = 37.5 \), and \( N_{\text{N2}} = 188 \).

\[ Q_{\text{out}} = (-249950) \left( \frac{kJ}{\text{kmol}_{\text{fuel}}} \right) - (456960) \left( \frac{kJ}{\text{kmol}_{\text{fuel}}} \right) \]
\[ \left( 8(-393520 + 28041) + 9(-241820 + 21924) + 37.5(19246) + 188(18221) \right) \]

\[ \rightarrow Q_{\text{out}} = (-249950 - 456960 + 755623) \left( \frac{kJ}{\text{kmol}_{\text{fuel}}} \right) \]

\[ \rightarrow Q_{\text{out}} = 48713 \left( \frac{kJ}{\text{kmol}_{\text{fuel}}} \right) \]