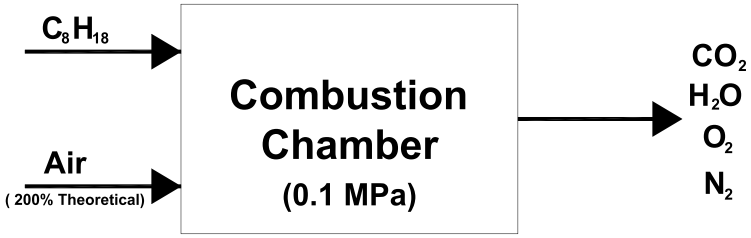
ME 354 Tutorial, Week#13
Reacting Mixtures

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 : $\rightarrow 18 = 2y$ So, $y = 9$
O : $\rightarrow 2\times 2\times b = 2x + y + 2b$ So, $b = 12.5$ (corrected)
N : $\rightarrow 2\times 2\times 3.76\times b = 2z$ So, $z = 94$ (corrected)

The balanced reaction equation is shown below in Eq1.

$$C_8H_{18} + 25(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 12.5O_2 + 94N_2 \text{ ......Eq 1}$$

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

N_{CO2} = 8 Kmole
N_{H2O} = 9 Kmole
N_{O2} = 12.5 Kmole
N_{N2} = 94 Kmole

$N_{products}$=(8+9+12.5+94)=123.5 Kmole

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

y_{CO2} = $N_{CO2}/N_{products}$ = (8/123.5) = 6.47%
y_{H2O} = $N_{H2O}/N_{products}$ = (9/123.5) = 7.29%
y_{O2} = $N_{O2}/N_{products}$ = (12.5/123.5) = 10.12%
Y_{N2} = $N_{N2}/N_{products}$ = (94/123.5) = 76.12%

Answer 1a)

[b] The air-Fuel Ratio, $AF = \dfrac{m_{AIR}}{m_{FUEL}} \left[\dfrac{Kg_{AIR}}{Kg_{FUEL}}\right]$ Eq.-2

$$m_{AIR} = N_{AIR} \times M_{AIR}$$

Where

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

$M_{AIR} = 29 \left[\dfrac{Kg_{AIR}}{Kmole}\right]$ {From Table A-2 of Text Book}

Similarly.

$$m_{FUEL} = N_{FUEL} \times M_{FIUEL}$$

Where

$N_{FUEL} = 1\,[Kmole]$ {From Balanced Reaction Equation}

$$M_{FUEL} = M_{C_2H_{18}} = (8 \times 12.012 + 18 \times 1.008) \left[\frac{Kg_{FUEL}}{Kmole} \right]$$

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_2O (i.e. the partial pressure of H_2O in the mixture). Since it is assumed that the combustion gases behave as ideal gases, the partial pressure of H_2O can be determined from the total pressure multiplied by the mole fraction of H_2O, y_{H2O}.

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

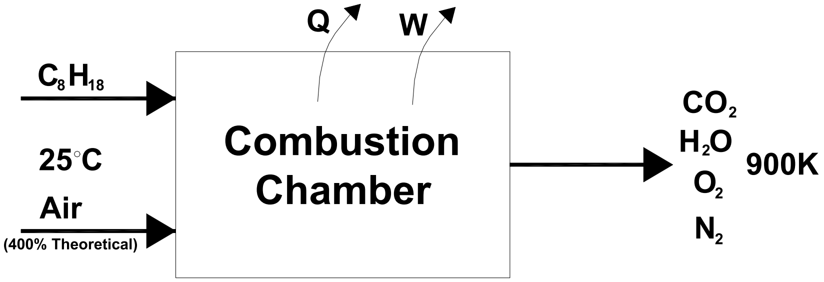
From Table A-4, interpolating in between 35°C and 40°C

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

Answer 1b)

Question 2:
A small gas turbine uses C_8H_{18} (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



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.

C's → $v_{O_2} = x = 8$

H_2's → $v_{H_2O} = \frac{y}{2} = \frac{18}{2} = 9$

O_2's → $v_{O_2} = x + \frac{y}{4} = 8 + \frac{18}{4} = 12.5$

N_2's → $v_{N_2} = 3.76(1+a)v_{O_2} = 3.76(4)(12.5) = 188$

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

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.

$$Q_{in} + W_{in} + \sum N_r(\bar{h}_f^\circ + \bar{h} - \bar{h}^\circ)_r = Q_{out} + W_{out} + \sum N_p(\bar{h}_f^\circ + \bar{h} - \bar{h}^\circ)_p \qquad \text{(Eq1)}$$

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_8H_{18}, O_2, and N_2)

Enthalpy of formation, $\bar{h}_f^\circ$

For stable elements O_2 and N_2, the enthalpy of formation is zero

$\rightarrow \bar{h}^\circ_{f\,O2}$ **= 0**

$\rightarrow \bar{h}^\circ_{f\,N2}$ **= 0**

The enthalpy of formation for C_8H_{18} (l), is found in Table A-26

$\rightarrow \bar{h}_f^\circ$ **= –249950 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.

$\rightarrow \left(\bar{h} - \bar{h}^\circ\right)_{O2}$ **=0**

$\rightarrow \left(\bar{h} - \bar{h}^\circ\right)_{N2}$ **=0**

$\rightarrow \left(\bar{h} - \bar{h}^\circ\right)_{C8H18}$ **=0**

Products (CO_2, H_2O, O_2, and N_2)

Enthalpy of formation, $\bar{h}_f^\circ$

For stable elements O_2 and N_2, the enthalpy of formation is zero

$\rightarrow \bar{h}^\circ_{f\,O2}$ ***= 0***

$\rightarrow \bar{h}^\circ_{f\,N2}$ ***= 0***

The enthalpy of formations for CO_2 and $H_2O(g)$, and located in Table A-26

$\rightarrow \bar{h}^{\circ}_{f\,CO2}$ **= –393520 kJ/kmol**

$\rightarrow \bar{h}^{\circ}_{f\,H2O}$ **= –241820 kJ/kmol**

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

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 $\bar{h}^{\circ}$) must be subtracted to ensure the enthalpies are all calculated with respect to the same reference state.

For CO_2,

$\rightarrow \bar{h}_{@900K}$ = 37405 kJ/kmol (Table A-20)

$\rightarrow \bar{h}^{\circ} = \bar{h}_{@298K}$ = 9364 kJ/kmol (Table A-20)

$\rightarrow \left(\bar{h} - \bar{h}^{\circ}\right)_{CO2}$ **= 28041 kJ/kmol**

For H_2O (g),

$\rightarrow \bar{h}_{@900K}$ = 31828 kJ/kmol (Table A-23)

$\rightarrow \bar{h}^{\circ} = \bar{h}_{@298K}$ = 9904 kJ/kmol (Table A-23)

$\rightarrow \left(\bar{h} - \bar{h}^{\circ}\right)_{H2O}$ **= 21924 kJ/kmol**

For O_2,

$\rightarrow \bar{h}_{@900K}$ = 27928 kJ/kmol (Table A-19)

$\rightarrow \bar{h}^{\circ} = \bar{h}_{@298K}$ = 8682 kJ/kmol (Table A-19)

$\rightarrow \left(\bar{h} - \bar{h}^{\circ}\right)_{O2}$ **= 19246 kJ/kmol**

For N_2,

$\rightarrow \bar{h}_{@900K}$ = 26890 kJ/kmol (Table A-18)

$\rightarrow \bar{h}^{\circ} = \bar{h}_{@298K}$ = 8669 kJ/kmol (Table A-18)

$\rightarrow \left(\bar{h} - \bar{h}^{\circ}\right)_{N2}$ **= 18221 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_{out} as shown below.

$$W_{out} = \frac{1\left[\frac{MJ}{s}\right]}{0.25\left[\frac{kg_{fuel}}{s}\right]} \times \frac{114.24\left[kg_{fuel}\right]}{1\left[kmol_{fuel}\right]} = 456.96\left[\frac{MJ}{kmol_{fuel}}\right] = 456960\left[\frac{kJ}{kmol_{fuel}}\right]$$

Note: The molar mass of C_8H_{18} was determined from the molar mass of C (12.012kg/kmol) and H (1.008kg/kmol)

$M_{fuel}=8(12.012)+18(1.008) = 114.24kg_{fuel}/kmol$.

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

$$Q_{out} = \sum N_r(\bar{h}_f^\circ + \Delta\bar{h})_r - W_{out} - \sum N_p(\bar{h}_f^\circ + \Delta\bar{h})_p \qquad \text{(Eq2)}$$

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: $N_{CO2}=8$, $N_{H2O}=9$, $N_{O2}=37.5$, and $N_{N2} = 188$.

$$Q_{out} = (-249950)\left[\frac{kJ}{kmol_{fuel}}\right] - (456960)\left[\frac{kJ}{kmol_{fuel}}\right]$$

$$-\begin{pmatrix} 8(-393520 + 28041) + 9(-241820 + 21924) \\ + 37.5(19246) + 188(18221) \end{pmatrix}$$

Answer 2)

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

$$\rightarrow Q_{out} = 48713\left[\frac{kJ}{kmol_{fuel}}\right]$$