1.1 Ethanol and dimethyl ether (DME) have been considered as potential fuels for the future and they are isomers. At ambient conditions, determine the phase of these two fuels.

Solution:
Ethanol: liquid; DME: gaseous

2.1 Consider an isentropic combustion system with a total of $K$ species. Assuming constant specific heats, show that the mixture temperature and pressure at two different states are related to the respective pressures as

$$
\frac{T_2}{T_1} = \left( \frac{P_2}{P_1} \right)^{(\gamma-1)/\gamma}
$$

where

$$
\gamma = \frac{\sum_i m_i c_{p,i}}{\sum_i m_i c_{v,i}}
$$

Solution:
Isentropic process leads to overall zero change of entropy

$$
\Delta S = \sum_{i=1}^K m_i \Delta s_i = \sum_{i=1}^K m_i \left( c_{p,i} \ln \frac{T_2}{T_1} - R_i \ln \frac{P_2}{P_1} \right) = 0
$$

$$
\sum_{i=1}^K m_i c_{p,i} \ln \frac{T_2}{T_1} = \sum_{i=1}^K m_i R_i \ln \frac{P_2}{P_1}
$$

$$
\ln \left( \frac{T_2}{T_1} \right)^{\sum_{i=1}^K m_i c_{p,i}} = \ln \left( \frac{P_2}{P_1} \right)^{\sum_{i=1}^K m_i R_i}
$$

$$
\frac{T_2}{T_1} = \left( \frac{P_2}{P_1} \right)^{\sum_{i=1}^K m_i c_{p,i} / \sum_{i=1}^K m_i c_{v,i}} = \left( \frac{P_2}{P_1} \right)^{\gamma (c_v - c_p) / c_v} = \left( \frac{P_2}{P_1} \right)^{(\gamma-1)/\gamma}
$$

where

$$
\gamma = \frac{\sum_{i=1}^K m_i c_{p,i}}{\sum_{i=1}^K m_i c_{v,i}}
$$
2.2 Measurements of exhaust gases from a methane-air combustion system show 3% of oxygen by volume (dry base) in the exhaust. Assuming complete combustion, determine the excess percentage of air, equivalence ratio, and fuel/air ratio.

Solution:
Using the overall reaction stoichiometric for methane in terms of normalized air/fuel ratio $\lambda$.

$$CH_4 + 2\lambda(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + \lambda \cdot 2 \cdot 3.76N_2 + 2(\lambda - 1)O_2$$

In the exhaust without water (dry base), the oxygen mole fraction is

$$x_{O_2} = \frac{2(\lambda - 1)}{1 + 7.52\lambda + 2(\lambda - 1)} = \frac{\%O_2}{100} \rightarrow \lambda = 1.15$$

Equivalence ratio (Eq. 2.16):

$$\phi = \frac{1}{\lambda} = 0.87$$

Percentage of excess air (see Table 2.1):

$$\%EA = 100 \frac{1 - \phi}{\phi} = 14.9\%$$

mass base fuel/air ratio (Eq. 2.15 or Table 2.1): $f = f_s \cdot \phi = \frac{M_f}{(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}) \cdot 4.76 \cdot M_{air} \cdot \phi} = \frac{16}{2 \cdot 4.76 \cdot 28.84 \cdot 0.87} = 0.051$

2.3 There has been a lot of interest about replacing gasoline with ethanol, but is this really a good idea? We’re going to compare a blend of ethanol (70% ethanol and 30% gasoline by volume) to gasoline. Calculate the lower heating value (LHV) of a 70% ethanol/30% isooctane mixture in terms of $kJ/mol$ of fuel. Assume complete combustion. How does this compare to the tabulated value for gasoline (isooctane)? Assuming a 20% thermal efficiency, if you need to get 100 kW of power from an engine, how much of each fuel (in mol/s) do you need? If you have a stoichiometric mixture of the ethanol/gasoline blend and air in your 100 kW engine, how much CO2 are you emitting in g/s? How does this compare to the same engine running a stoichiometric mixture of 100% gasoline and air?

Solution:

$$0.7C_2H_5OH + 0.3C_8H_{18} + x(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2$$

C balance:
$0.7 \cdot 2 + 0.3 \cdot 8 = a$

$a = 3.8$

H balance:

$0.7 \cdot 6 + 0.3 \cdot 18 = 2b$

$b = 4.8$

O balance:

$0.7 + 2x = 2a + b$

$0.7 + 2x = 2 \cdot 3.8 + 4.8$

$x = 5.85$

$0.7C_2H_5OH + 0.3C_8H_{18} + 5.85(O_2 + 3.76N_2) \rightarrow 3.8CO_2 + 4.8H_2O + 22N_2$

Using Eq. 2.26:

$LHV = -Q_{\text{run,p}}^0 = \sum N_{i,R} \Delta h_{i,R}^0 - \sum N_{i,p} \Delta h_{i,p}^0$

$LHV = 0.7\Delta h_{C_2H_5OH}^0 + 0.3\Delta h_{C_8H_{18}}^0 - (3.8\Delta h_{CO_2}^0 + 4.8\Delta h_{H_2O}^0)$

$LHV = 0.7(-235.1 \frac{MJ}{kmol}) + 0.3(-259.2 \frac{MJ}{kmol})$

$- \left[3.8(-393.52 \frac{MJ}{kmol}) + 4.8(-241.83 \frac{MJ}{kmol}) \right]$

$LHV = 2413.83 \frac{MJ}{kmol} = 2413.83 \frac{kJ}{mol}$

The tabulated LHV for isoctane is 44,651 kJ/kg, or

$44,651 \frac{kJ}{kg} \cdot \frac{114.23 kg}{1 \text{kmol}} \cdot \frac{1 \text{kmol}}{1000 \text{mol}} = 5,100.48 \frac{kJ}{mol}$

so the LHV of plain gasoline is about two times greater than the mixture. To get 100kW of power from an engine with 20% efficiency, you’d need:

mixture: $100kW = 100 \frac{kJ}{s} \cdot \frac{1 \text{molfuel}}{2413.83kJ} \cdot \frac{1}{0.2} = 0.207 \frac{mol}{s}$

gasoline: $100kW = 100 \frac{kJ}{s} \cdot \frac{1 \text{molfuel}}{5100.48kJ} \cdot \frac{1}{0.2} = 0.098 \frac{mol}{s}$

By looking at the stoichiometry above, an engine running the fuel mixture will produce 3.8 mol of CO2 per mol of fuel burned. The emissions are then

$CO_{2,\text{gen}} = \frac{3.8 \text{molCO}_2}{1 \text{molfuel}} \cdot \frac{0.207 \text{molfuel}}{s} = 0.787 \frac{molCO_2}{s} \cdot \frac{44g}{mol} = 34.64 \frac{g}{s}$

For gasoline, assuming isoctane,

$C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 47N_2$

so 1 mol of isoctane produces 8 mol of CO2 and the emission rate is:

$CO_{2,\text{gen}} = \frac{8 \text{molCO}_2}{1 \text{molfuel}} \cdot \frac{0.098 \text{molfuel}}{s} = 0.784 \frac{molCO_2}{s} \cdot \frac{44g}{mol} = 34.51 \frac{g}{s}$

The emission rate of CO2 is virtually the same for the two fuels.
2.4 Gasoline is assumed to have a chemical composition of C\textsubscript{8.26}H\textsubscript{15.5}.

a) Determine the mole fractions of CO\textsubscript{2} and O\textsubscript{2} in the exhaust for an engine with normalized air/fuel ratio $\lambda = 1.2$ with the assumption of complete combustion.

b) The enthalpy of formation of C\textsubscript{8.26}H\textsubscript{15.5} is –250 MJ/kmol. Determine the LHV of gasoline in terms of MJ/kg. The molecular mass of C\textsubscript{8.26}H\textsubscript{15.5} is 114.62 kg/kmol.

c) Using an average $c_p$ for the products at 1,200 K, estimate the adiabatic flame temperature at constant pressure of 1 atm for the lean ($\lambda = 1.2$) mixture.

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Solutions:

\[ C_\alpha H_\beta O_\gamma + \lambda (\alpha + \frac{\beta}{4} - \frac{\gamma}{2}) (O_2 + 3.76 N_2) \]

\[ \rightarrow \alpha CO_2 + \frac{\beta}{2} H_2 O + \lambda (\alpha + \frac{\beta}{4} - \frac{\gamma}{2}) N_2 + (\alpha + \frac{\beta}{4} - \frac{\gamma}{2})(\lambda - 1) O_2 \]

with $\alpha = 8.26$, $\beta = 15.5$, and $\gamma = 0$, we have

\[ C_{8.26}H_{15.5} + \lambda \cdot 12.135 \cdot (O_2 + 3.76 N_2) \]

\[ \rightarrow 8.26 \cdot CO_2 + 7.75 \cdot H_2 O + \lambda \cdot 45.63 N_2 + 12.135 \cdot (\lambda - 1) O_2 \]

with $\lambda = 1.2$

\[ C_{8.26}H_{15.5} + 14.562 \cdot (O_2 + 3.76 N_2) \]

\[ \rightarrow 8.26 \cdot CO_2 + 7.75 \cdot H_2 O + 54.756 N_2 + 2.427 \cdot O_2 \]

\[ x_{CO_2} = \frac{8.26}{8.26 + 7.75 + 54.756 + 2.427} = 0.113 \]

\[ x_{O_2} = \frac{2.427}{8.26 + 7.75 + 54.756 + 2.427} = 0.033 \]

b) Using Eq. 2.27, LHV for a constant pressure reactor at STD is

\[ LHV = \frac{-250 MJ/kmol - \left[ 8.26(-393.52) + 7.75(-241.83) \right] MJ/kmol}{114.62 kg/kmol} = 42.53 MJ/kg \]

Note that the enthalpy formation for H\textsubscript{2}O(g) is used instead of H\textsubscript{2}O(liq).