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

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

Solution:
Isentropic process leads to overall zero change of entropy

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

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

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

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

$$\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{\sum_{i=i}^{K} m_i R_i / \sum_{i=1}^{K} m_i c_{p_i}} = \left(\frac{P_2}{P_1}\right)^{\sum_{i=i}^{K} m_i (c_{p_i} - c_{vi}) / \sum_{i=1}^{K} m_i c_{p_i}} = \left(\frac{P_2}{P_1}\right)^{(\gamma-1)/\gamma}$$

where $\gamma = \dfrac{\sum_{i=1}^{K} m_i c_{p,i}}{\sum_{i=1}^{K} m_i c_{v,i}}$

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 ration λ

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

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

$$x_{O2} = \frac{2(\lambda - 1)}{1 + 7.52\lambda + 2(\lambda - 1)} = \frac{\%O_2}{100} \rightarrow \lambda = 1.15$$

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 CO_2 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:

$$LHV = -Q^0_{rxn,p} = \sum N_{i,R}\Delta h^o_{i,R} - \sum N_{i,P}\Delta h^o_{i,P}$$

$$LHV = 0.7\Delta h^o_{C_2H_5OH} + 0.3\Delta h^o_{C_8H_{18}} - \left(3.8\Delta h^o_{CO_2} + 4.8\Delta h^o_{H_2O}\right)$$

$$LHV = 0.7\left(-235.1\, {}^{MJ}\!/\!{}_{kmol}\right) + 0.3\left(-259.2\, {}^{MJ}\!/\!{}_{kmol}\right)$$
$$-\left[3.8\left(-393.52\, {}^{MJ}\!/\!{}_{kmol}\right) + 4.8\left(-241.83\, {}^{MJ}\!/\!{}_{kmol}\right)\right]$$

$$LHV = 2413.83\, {}^{MJ}\!/\!{}_{kmol} = 2413.83\, {}^{kJ}\!/\!{}_{mol}$$

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

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

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

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

By looking at the stoichiometry above, an engine running the fuel mixture will produce 3.8 mol of CO_2 per mol of fuel burned. The emissions are then

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

For gasoline, assuming isooctane,

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

so 1 mol of isooctane produces 8 mol of CO_2 and the emission rate is:

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

The emission rate of CO_2 is virtually the same for the two fuels.

2.4 Gasoline is assumed to have a chemical composition of $C_{8.26}H_{15.5}$.

a) Determine the mole fractions of CO_2 and O_2 in the exhaust for an engine with normalized air/fuel ratio λ = 1.2 with the assumption of complete combustion.

b) The enthalpy of formation of $C_{8.26}H_{15.5}$ is –250 *MJ/kmol*. Determine the LHV of gasoline in terms of *MJ/kg*. The molecular mass of $C_{8.26}H_{15.5}$ 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 (λ = 1.2) mixture.

Solutions:

a)
$$C_\alpha H_\beta O_\gamma + \lambda(\alpha + \frac{\beta}{4} - \frac{\gamma}{2})(O_2 + 3.76N_2)$$
$$\rightarrow \alpha CO_2 + \frac{\beta}{2}H_2O + \lambda \cdot 3.76(\alpha + \frac{\beta}{4} - \frac{\gamma}{2})N_2 + (\alpha + \frac{\beta}{4} - \frac{\gamma}{2})(\lambda - 1)O_2$$

with α=8.26, β=15.5, and γ=0, we have

$$C_{8.26}H_{15.5} + \lambda \cdot 12.135 \cdot (O_2 + 3.76N_2)$$
$$\rightarrow 8.26 \cdot CO_2 + 7.75 \cdot H_2O + \lambda \cdot 45.63N_2 + 12.135 \cdot (\lambda - 1)O_2$$

with $\lambda = 1.2$

$$C_{8.26}H_{15.5} + 14.562 \cdot (O_2 + 3.76N_2)$$
$$\rightarrow 8.26 \cdot CO_2 + 7.75 \cdot H_2O + 54.756N_2 + 2.427 \cdot O_2$$

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

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

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

$$LHV = \frac{\sum_i N_{i,R}\Delta\hat{h}_{i,R}(T_0) - \sum_i N_{i,P}\Delta\hat{h}_{i,P}(T_0)}{N_{fuel}M_{fuel}}$$

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

Note that the enthalpy formation for $H_2O(g)$ is used instead of $H_2O(liq)$.