

**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

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

Solution:

Isentropic process leads to overall zero change of entropy

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

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

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

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

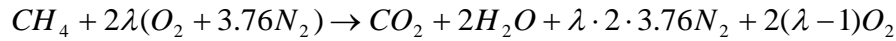
$$\frac{T_2}{T_1} = \left( \frac{P_2}{P_1} \right)^{\frac{\sum_{i=1}^K m_i R_i}{\sum_{i=1}^K m_i c_{p,i}}} = \left( \frac{P_2}{P_1} \right)^{\frac{\sum_{i=1}^K m_i (c_{p,i} - c_{v,i})}{\sum_{i=1}^K m_i c_{p,i}}} = \left( \frac{P_2}{P_1} \right)^{(\gamma-1)/\gamma}$$

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  $\lambda$



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):

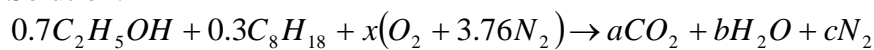
$$\%EA = 100 \frac{1 - \phi}{\phi} = 14.9\%$$

mass base fuel/air ratio (Eq. 2.15 or Table 2.1):  $f = f_s \cdot \phi =$

$$\frac{M_f}{\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right) \cdot 4.76 \cdot M_{air}} \cdot \phi = \frac{16}{2 \cdot 4.76 \cdot 28.84} \cdot 0.87 = 0.051$$

**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:



C balance:

Solutions for *Fundamentals of Combustion Processes*

$$0.7 \cdot 2 + 0.3 \cdot 8 = a$$

$$a = 3.8$$

H balance:

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

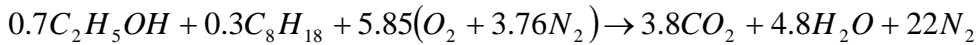
$$b = 4.8$$

O balance:

$$0.7 + 2x = 2a + b$$

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

$$x = 5.85$$



Using Eq. 2.26:

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

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

$$LHV = 0.7(-235.1 \text{ MJ/kmol}) + 0.3(-259.2 \text{ MJ/kmol}) - [3.8(-393.52 \text{ MJ/kmol}) + 4.8(-241.83 \text{ MJ/kmol})]$$

$$LHV = 2413.83 \text{ MJ/kmol} = 2413.83 \text{ kJ/mol}$$

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

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

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:

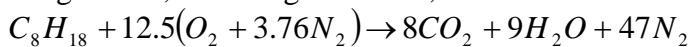
$$\text{mixture: } 100 \text{ kW} = 100 \frac{\text{kJ}}{\text{s}} \cdot \frac{1 \text{ mol fuel}}{2413.83 \text{ kJ}} \cdot \frac{1}{0.2} = 0.207 \frac{\text{mol}}{\text{s}}$$

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

By looking at the stoichiometry above, an engine running the fuel mixture will produce 3.8 mol of CO<sub>2</sub> per mol of fuel burned. The emissions are then

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

For gasoline, assuming isooctane,



so 1 mol of isooctane produces 8 mol of CO<sub>2</sub> and the emission rate is:

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

The emission rate of CO<sub>2</sub> is virtually the same for the two fuels.

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

- Determine the mole fractions of  $CO_2$  and  $O_2$  in the exhaust for an engine with normalized air/fuel ratio  $\lambda = 1.2$  with the assumption of complete combustion.
- The enthalpy of formation of  $C_{8.26}H_{15.5}$  is  $-250 \text{ MJ/kmol}$ . Determine the LHV of gasoline in terms of  $\text{MJ/kg}$ . The molecular mass of  $C_{8.26}H_{15.5}$  is  $114.62 \text{ kg/kmol}$ .
- 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.

Solutions:

$$\begin{aligned} & C_{\alpha}H_{\beta}O_{\gamma} + \lambda\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)(O_2 + 3.76N_2) \\ \text{a)} \quad & \rightarrow \alpha CO_2 + \frac{\beta}{2}H_2O + \lambda \cdot 3.76\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)N_2 + \left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)(\lambda - 1)O_2 \end{aligned}$$

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

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

with  $\lambda = 1.2$

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

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

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

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

$$\begin{aligned} LHV &= \frac{\sum_i N_{i,R} \hat{\Delta} h_{i,R}(T_0) - \sum_i N_{i,P} \hat{\Delta} h_{i,P}(T_0)}{N_{fuel} M_{fuel}} \\ &= \frac{-250 \text{ MJ / kmol} - [8.26(-393.52) + 7.75(-241.83)] \text{ MJ / kmol}}{114.62 \text{ kg / kmol}} = 42.53 \text{ MJ / kg} \end{aligned}$$

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