2.62 – Advanced Energy Conversion | Spring 2020

Homework 2 – Solutions

Problem 1

a) **For each fuel, calculate the required fuel flow rate and CO2 emission rate. Explain their relative values, and comment on which is the best fuel and why. [10 points]**

The powerplant's power rating is 100 MWe and the first law efficiency is 35% = 0.35, which means that the heat input to the plant is 100/0.35 = 286 MW in each case.

Since the efficiency of the power plant is based on the lower heating value (LHV) of the fuels, the first thing to do is to find out the LHV of each fuel considered. NIST webbook is used here as reference for LHV of fuels (If you are interested in a deeper analysis of heating values of fuel, you can check Chase (1998), which is also used by NIST webbook as reference for heating values of hydrocarbons.) The molar mass of CO_2 is 44 g/mol.
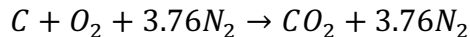
For each fuel, we should calculate the required fuel flow rate and CO_2 emissions.

(i)   **Lignite (C):**

LHV of lignite is 15 MJ/kg and the molar mass is 12 g/mol (we neglect the other components in lignite). In ideal conditions, the required lignite flow rate is:

$$\frac{286}{15} = 19 \text{ kg/s} \quad \text{or} \quad \frac{19000}{12} = 1583.3 \text{ mol/s}$$

The combustion reaction for lignite is:

$$C + O_2 + 3.76N_2 \rightarrow CO_2 + 3.76N_2$$

Therefore, the stoichiometric and complete combustion of 1 mole of lignite forms 1 mole of CO_2 and CO_2 emission is:
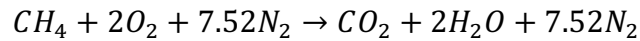
$$1583.3 \times 0.044 = 69.67 \text{ kg/s}$$

1

(ii)   **Methane (CH₄):**

The LHV of methane is 50 MJ/kg and the molar mass is 16 g/mol. In ideal conditions, the required methane flow rate is:

$$\frac{286}{50} = 5.72 \text{ kg/s} \quad \text{or} \quad \frac{5720}{16} = 357.5 \text{ mol/s}$$

The combustion reaction for methane is:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2$$

Therefore, the stoichiometric and complete combustion of 1 mole of methane forms 1 mole of CO_2 and the emission rate of CO_2 is:
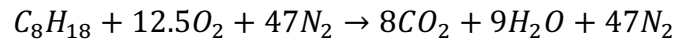
$$357.5 \times 0.044 = 15.73 \text{ kg/s}$$

(iii)   **Octane (C₈H₁₈):**

LHV of octane is 45 MJ/kg and the molar mass is 114 g/mol. In ideal conditions, the required flow rate is:

$$\frac{286}{45} = 6.36 \text{ kg/s} \quad \text{or} \quad \frac{6360}{114} = 55.75 \text{ mol/s}$$

The combustion reaction for octane is:

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

Therefore, stoichiometric and complete combustion of 1 mole of octane forms 8 moles of CO_2 and the CO_2 emission rate is:

$$55.75 \times 8 \times 0.044 = 19.624 \text{ kg/s}$$

As the results show us, the require flow rate is the largest in the case of lignite and the lowest in the case of methane, as a direct consequence of the LHV. In terms of the amount of the fuel required, the order from most to least is lignite, octane, and methane. The same order is valid for CO_2 emission from most to least. The CO_2 emissions of methane and octane are close, while that of lignite is around 4 times higher, which shows lignite is the dirtiest fuel among these three regarding global warming potential.

b) Is it reasonable to assume the same efficiency for all fuels? Why? [2.5 points]

It is not reasonable to assume the same efficiency for all fuels. It is easy to verify that each fuel has a different adiabatic flame temperature. Therefore, even if we assume a similar power cycle for all fuels, they will result in different efficiencies (see discussion in notes). Note also that CH_4 can be directly used in a combined cycle which is more efficient.

c) Now keep the efficiency the same for lignite but take 52% for octane and 58% for methane. Calculate CO_2 emissions as kgCO₂/MJe for each fuel. [5 points]

- **Lignite (C):**

$$\frac{69.67 \text{kg/s}}{100 \text{ MWe}} = 0.6967 \text{ kgCO}_2/\text{MJe}$$

- **Methane (CH_4):**

$$\frac{\left(\frac{100}{0.58}\right)}{50} = 3.45 \text{ kg/s} \quad \text{or} \quad \frac{3450}{16} = 215.6 \text{ mol/s of fuel}$$

$$215.6 \times 0.044 = 9.49 \text{ kg/s CO}_2$$

$$\frac{9.49 \text{ kg/s}}{100 \text{ MWe}} = 0.0949 \text{ kgCO}_2/\text{MJe}$$

- **Octane (C_8H_{18}):**

$$\frac{\left(\frac{100}{0.52}\right)}{45} = 4.27 \text{ kg/s} \quad \text{or} \quad \frac{4270}{114} = 37.46 \text{ mol/s of fuel}$$

$$37.46 \times 8 \times 0.044 = 13.19 \text{ kg/s CO}_2$$

$$\frac{13.19 \text{ kg/s}}{100 \text{ MWe}} = 0.132 \text{ kgCO}_2/\text{MJe}$$

d) **The plant runs at 75% capacity factor, calculate the total CO2 emitted yearly from each plant, in kgCO₂. [5 points]**

At 75% capacity, the plant now generates 75 MWe. Using the efficiencies specified in part c, we calculate the carbon emissions (CE) as shown:

(i)   **Lignite (C):**

$$CE = 0.6967 \text{ kg CO}_2/\text{MJe} \times 0.75 \times 100 \text{ MWe} \times 3600 \times 24 \times 365$$

$$= 1.65 \times 10^9 \text{ kg CO}_2/\text{yr}$$

(ii)   **Methane (CH₄):**

$$CE = 0.0949 \text{ kg CO}_2/\text{MJe} \times 0.75 \times 100 \text{ MWe} \times 3600 \times 24 \times 365$$

$$= 0.224 \times 10^9 \text{ kg CO}_2/\text{yr}$$

Octane (C₈H₁₈):

$$CE = 0.132 \text{ kg CO}_2/\text{MJe} \times 0.75 \times 100 \text{ MWe} \times 3600 \times 24 \times 365$$

$$= 0.312 \times 10^9 \text{ kg CO}_2/\text{yr}$$

Now for methane only:
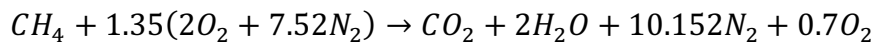
e) **Calculate the adiabatic flame temperature assuming air excess of 35% and that the reaction is complete: [7.5 points]**

Assuming an air excess of 35%, the combustion reaction has the form:

$$CH_4 + 1.35(2O_2 + 7.52N_2) \rightarrow CO_2 + 2H_2O + 10.152N_2 + 0.7O_2$$

We also assume complete combustion occurs in an adiabatic chamber, so the first law gives:

$$\sum_i \dot{n}_{i,in}\hat{h}_{i,in} = \sum_i \dot{n}_{i,out}\hat{h}_{i,out}$$

where i denotes the species and $\dot{n}_i$ is the molar flowrate of this species. We rewrite this equation as follows:

$$\dot{n}_{CH_4,in}\hat{h}_{CH_4,in} + \dot{n}_{O_2,in}\hat{h}_{O_2,in} + \dot{n}_{N_2,in}\hat{h}_{N_2,in} = \dot{n}_{CO_2,out}\hat{h}_{CO_2,out} + \dot{n}_{H_2O,out}\hat{h}_{H_2O,out} + \dot{n}_{O_2,out}\hat{h}_{O_2,out} + \dot{n}_{N_2,out}\hat{h}_{N_2,out}$$

The formation energies of these species can be found in NIST Chemistry WebBook (They use 298.15 K as standard temperature here):

$$H^{\circ}_{f,CH_4} = -74.87 \text{ kJ/mol} \qquad H^{\circ}_{f,O_2} = 0 \text{ kJ/mol} \qquad H^{\circ}_{f,N_2} = 0 \text{ kJ/mol}$$

$$H^{\circ}_{f,H_2O} = -241.8 \text{ kJ/mol} \qquad H^{\circ}_{f,CO_2} = -393.5 \text{ kJ/mol}$$

Given the large range of temperature changes from inlet to adiabatic temperature, it is not good practice to assume constant heat capacities for the gases. Therefore, using the equation in NIST Chemistry WebBook, we have the enthalpy relations of the gases:

$$H^{\circ} - H^{\circ}_{298.15K} = A \cdot t + \frac{B}{2} \cdot t^2 + \frac{C}{3} \cdot t^3 + \frac{D}{4} \cdot t^4 - \frac{E}{t} + F - H \quad [\text{kJ/mol}]$$

where $t = T[K]/1000$, and the constants are:

	CO_2	O_2	N_2	H_2O
T (K)	1200 − 6000	2000 − 6000	2000 − 6000	1700 − 6000
A	58.16639	20.911	35.519	41.964
B	2.720074	10.721	1.1287	8.6221
C	-0.492289	-2.02	-0.196	-1.5
D	0.038844	0.1464	0.0147	0.0981
E	-6.447293	9.2457	-4.554	-11.16
F	-425.9186	5.3377	-18.97	-272.2
H	-393.5224	0	0	-241.8

$$1 \cdot H^{\circ}_{f,CH_4} = 1 \cdot \left(H^{\circ}_{f,CO_2} + H_{CO_2}(T)\right) + 2 \cdot \left(H^{\circ}_{f,H_2O} + H_{H_2O}(T)\right) + 0.7 \cdot H_{O_2}(T) + 10.152 \cdot H_{N_2}(T)$$

Plugging-in and solving for T:

$$T = 1917 \text{ K}$$

f) **Based on the adiabatic flame temperature and that of the environment, calculate a maximum first law efficiency using the standard "Carnot efficiency". [2.5 points]**

The standard "Carnot efficiency" is stated as:

$$\eta_{carnot} = 1 - \frac{T_0}{T_H}$$

where T_0 is the standard ambient temperature (*environment is usually the cold reservoir*) and T_H is the hot reservoir temperature. Here, we use the adiabatic flame temperature to be T_H, which gives:

$$\eta_{carnot} = 1 - \frac{T_0}{T_H} = 1 - \frac{298}{1917} = 84.5\%$$

g) **Correct the efficiency to account for the fact that the heat source has finite flowrate, and to allow for a 10K temperature difference between the source, the heat engine and the environment. [2.5 points]**

If the heat source has finite flow rate and the corrected Carnot efficiency can be defined as:

$$\eta_{carnot^*} = 1 - \frac{\ln\left(\frac{T_H}{T_C}\right)}{\frac{T_H}{T_C} - 1}$$

where T_H is the adiabatic flame temperature, and T_C is 298 + 10 = 308 K, since we allow for a 10K temperature difference for the removal of heat to the environment. Therefore:

$$\eta_{carnot^*} = 1 - \frac{\ln\left(\frac{T_H}{T_C}\right)}{\frac{T_H}{T_C} - 1} = 1 - \frac{\ln\left(\frac{1917}{308}\right)}{\frac{1917}{308} - 1} = 65\%$$

Since we account for the finite flowrate and higher outlet temperature, this efficiency is lower than the ideal case addressed previously.

h) **What is the second law efficiency of this plant? [5 points]**

First, we need to find the heat extracted from the exhaust stream:

$$Q_H = \sum n_i \hat{h}_{i,out} - \sum n_i \hat{h}_{i,in}$$

$$Q_H = n_{CO_2}\hat{h}_{CO_2,out} + n_{H_2O}\hat{h}_{H_2O,out} + n_{N_2}\hat{h}_{N_2,out} + n_{O_2}\hat{h}_{O_2,out}$$
$$- \left(n_{CO_2}\hat{h}_{CO_2,in} + n_{H_2O}\hat{h}_{H_2O,in} + n_{N_2}\hat{h}_{N_2,in} + n_{O_2}\hat{h}_{O_2,in}\right)$$

Calculating Q_H (per mole of CH_4) using the definition in Part e:

$$Q_H = 700.8 \text{ kJ}$$

Accounting for the efficiency of the plant from Part g:

$$W_{ideal} = \eta_{carnot} Q_H = 0.845 \times 700.8 = 592.176 \text{ kJ}$$

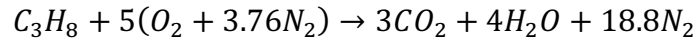The actual work of the plant (specified in Part c) per mole of CH_4 is:

$$W_{actual} = \eta_I Q_H = 0.58 \times 700.8 = 406.464 \text{ kJ}$$

Therefore:

$$\eta_{II} = \frac{W_{actual}}{W_{ideal}} = \frac{406.464}{592.176} = 68.6\%$$

Problem 2

The chemical equation for stochiometric combustion is air is given by: **[5 points]**

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$

Accounting for isentropic compression (and keeping in mind the composition is assumed frozen), the temperature of the compressed mixture is given by:

$$\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{1-1/\gamma} = (20)^{1-\frac{1}{1.4}} = 2.35$$

Therefore:

$$T_2 = 2.35T_1 = 2.35 \times 298 = 701K$$

a) **Calculate the products' temperature without dissociation. [10 points]**

The adiabatic flame temperature may be computed through the conservation of enthalpy:

$$H_R = H_P$$

$$\sum_{react} n_i \hat{h}_i = \sum_{products} n_i \hat{h}_i$$

Taking the temperature of the reactants to be 701 K, and using EES:

Equations Window
"Given: Propane combustion at initial conditions of 2 MPa and 701 K"
"Find: adiabatic flame temperature"
"Solution:"
"1) combustion stoichiometry
C3H8 + 5 (O2 + 3.76 N2) ===> 3 CO2 + 4 H2O + 18.8 N2
2) enthalpy of reactants"
T_o = 701
h_R = ENTHALPY(C3H8,T=T_o) + 5 * ENTHALPY(O2,T=T_o) + 18.8 * ENTHALPY(N2,T=T_o)
"3) enthalpy of products"
h_P = 3 * ENTHALPY(CO2,T=T_a) + 4 * ENTHALPY(H2O,T=T_a) + 18.8 * ENTHALPY(N2,T=T_a)
"4) energy balance"
h_R = h_P

Therefore:

$$T_{ad} = 2695.3 \text{ K}$$

b) **Calculate the products' composition and temperature with dissociation. [15 points]**

Now with dissociation, the combustion reaction takes the form:

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dO_2 + eN_2 + fH_2 + gCO$$
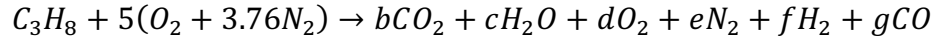
Applying mass balances:

C: b + g = 3   **H:** 2c + 2f = 8   **O:** 2b + c + 2d + g = 10   **N:** 2e = 37.6

Note this gives us four equations for 6 unknowns. To solve the system, we need two more equations. We use the dissociation reactions:

$$CO_2 \leftrightarrow CO + \frac{1}{2}O_2 \qquad\qquad H_2O + CO \leftrightarrow H_2 + CO_2$$

Using the definition of equilibrium constant:

$$\frac{P_{CO}P_{O_2}^{1/2}}{P_{CO_2}} = K_{p1} \quad\rightarrow\quad \frac{X_{CO}X_{O_2}^{1/2}}{X_{CO_2}} = K_{p1}\sqrt{p} \quad\rightarrow\quad \frac{gd^{1/2}}{b[b+c+d+e+f+g]^{1/2}} = \frac{K_{p1}}{\sqrt{p}}$$

$$\frac{P_{CO_2}P_{H_2}}{P_{CO}P_{H_2O}} = K_{p2} \quad\rightarrow\quad \frac{X_{CO_2}X_{H_2}}{X_{CO}X_{H_2O}} = K_{p2} \quad\rightarrow\quad \frac{bf}{gc} = K_{p2}$$

Assuming a temperature of 2000 K and referring to the notes:

$$K_{p1} = 10^{-2.884} = 0.0013 \qquad\qquad K_{p2} = 10^{-0.656} = 0.2208$$

Using EES, we solve the system of 6 equations and arrive at the following:

$b = 2.969$ $c = 3.991$ $d = 0.02016$ $e = 18.8$ $f = 0.009228$ $g = 0.03109$

Next, we calculate the temperature in EES as in part (a):

$$T = 2685.49 \text{ K}$$

Updating our guess to T = 2600 K, and doing another iteration (to confirm convergence), we arrive at the following:

$$K_{p1} = 10^{-1.219} = 0.06 \qquad\qquad K_{p2} = 10^{-0.802} = 0.158$$

Using EES, we solve the system of 6 equations and arrive at the following:

$$b = 2.625 \qquad c = 3.912 \qquad d = 0.232 \qquad e = 18.8 \qquad f = 0.08842 \qquad g = 0.3755$$

Next, we calculate the temperature in EES as in part (a):

$$T = 2581.047 \text{ K}$$

Of course, this iterative process can be repeated until a smaller tolerance is reached.

c) **Repeat (a) and (b) for the case when the original fuel-air mixture undergoes volume reduction to 1/10th of its original volume (with frozen composition) then constant volume combustion: [15 points]**

Again, the chemical equation for stochiometric combustion is air is given by:

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$
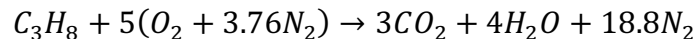
Accounting for **adiabatic compression** (and keeping in mind the composition is assumed frozen), the temperature of the compressed mixture is given by:

$$\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} = (10)^{0.4} = 2.512$$

Therefore:

$$T_2 = 2.35T_1 = 2.512 \times 298 = 748.5 \text{ K}$$

The adiabatic flame temperature without dissociation may be computed through the conservation of enthalpy (as done previously):

$$H_R = H_P$$

$$\sum_{react} n_i \hat{h}_i = \sum_{products} n_i \hat{h}_i$$

Taking the temperature of the reactants to be 748.5 K, and using EES:

$$T_{ad} = 2733.9 \text{ K}$$

As we can see, adiabatic compression and constant volume combustion lead to higher adiabatic flame temperatures than isentropic compression and constant pressure combustion.

Assuming T = 2600 K, we arrive at the following:

$$K_{p1} = 10^{-1.219} = 0.06 \qquad\qquad K_{p2} = 10^{-0.802} = 0.158$$

Using EES, we solve the system of 6 equations and arrive at the following:

$b = 2.625 \qquad c = 3.912 \qquad d = 0.232 \qquad e = 18.8 \qquad f = 0.08842 \qquad g = 0.3755$

Next, we calculate the temperature in EES as in part (a):

$$T = 2619 \text{ K}$$

Of course, this iterative process can be repeated until a smaller tolerance is reached.

Problem 3

a) If the combustion is stoichiometric, calculate the temperature of products assuming complete combustion. [10 points]

Technology one: Combustion

a) If the combustion of biomass is stoichiometric, then the combustion reaction has the form:

$$C_6H_{12}O_6 + 6(O_2 + 3.76N_2) \rightarrow 6CO_2 + 6H_2O + 22.56N_2$$
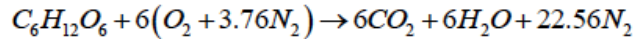
Assuming complete combustion occurs in an adiabatic chamber, we can write the first law as follows:

$$n_{C_6H_{12}O_6}\hat{h}_{C_6H_{12}O_6,in} + n_{O_2}\hat{h}_{O_2,in} + n_{N_2}\hat{h}_{N_2,in} = n_{CO_2}\hat{h}_{CO_2,out} + n_{H_2O}\hat{h}_{H_2O,out} + n_{N_2}\hat{h}_{N_2,out}$$

Biomass and air enter the combustion chamber at atmospheric conditions, therefore:

$$n_{C_6H_{12}O_6}\hat{h}_{C_6H_{12}O_6,in} = n_{CO_2}\hat{h}_{CO_2,out} + n_{H_2O}\hat{h}_{H_2O,out} + n_{N_2}\hat{h}_{N_2,out}$$

where for material i,

$$\hat{h}_i(T) = \hat{h}_{f,i}^o + \int_{T_o}^{T} \hat{c}_{p,i}dT$$

$$\hat{c}_{p,i} = a_i \Rightarrow \hat{h}_i(T) = \hat{h}_{f,i}^o + a_i(T - T_o)$$

Using this, we can determine the enthalpy values as:

$$\hat{h}_{C_6H_{12}O_6,in} = -1267.1 \; kJ/mol$$

$$\hat{h}_{CO_2,out} = -393.8 + 50.6(T_{out} - 298) \; kJ/mol$$

$$\hat{h}_{H_2O,out} = -242 + 38.2(T_{out} - 298) \; kJ/mol$$

$$\hat{h}_{N_2,out} = -31.1(T_{out} - 298) \; kJ/mol$$

Hence, per mole of biomass,

$$-1267.1 = 6(-393.8 + 50.6(T_{out} - 298)) + 6(-242 + 38.2(T_{out} - 298)) + 22.56(-31.1(T_{out} - 298))$$

Solving, we get $T_{out} = 2359.7 \; K$

b) **Calculate the maximum possible efficiency for the system, and maximum efficiency of the power cycle (both based on the logarithmic mean temperature). [5 points]**

b) Now, we know that:

$$\eta_{car} = 1 - \frac{\ln\left(\dfrac{T_F}{T^*}\right)}{\dfrac{T_F}{T^*} - 1}$$

For the steam cycle, $T^* = T_{ambient} = 298\ K$ and $T_F = T_{turb\_max} = 823\ K$. In addition, for the overall system, $T^* = T_C = 323\ K$ and $T_F = T_{products} = 2359.7\ K$. Substituting, we get the maximum possible efficiencies of the system and steam cycle:

$$\eta_{sys} = 1 - \frac{\ln\left(\dfrac{2359.7}{323}\right)}{\dfrac{2359.7}{323} - 1} = 0.684 = 68.4\%$$

$$\eta_{steam\_cycle} = 1 - \frac{\ln\left(\dfrac{823}{298}\right)}{\dfrac{823}{298} - 1} = 0.423 = 42.3\%$$

c) **If the second law efficiency of the power cycle is 60%, calculate the work produced by the plant per mole of biomass. [10 points]**

c) First, we have to find the amount of heat addition to the steam cycle:

$$Q_H = \sum n_i \hat{h}_{i,out} - \sum n_i \hat{h}_{i,in}$$

$$\Rightarrow Q_H = n_{CO_2}\hat{h}_{CO_2,out} + n_{H_2O}\hat{h}_{H_2O,out} + n_{N_2}\hat{h}_{N_2,out} - \left(n_{CO_2}\hat{h}_{CO_2,in} + n_{H_2O}\hat{h}_{H_2O,in} + n_{N_2}\hat{h}_{N_2,in}\right)$$

Hence, per mole of biomass, we get:

$$Q_H = 6\left(50.6\left(2359.7 - 323\right)\right) + 6\left(38.2\left(2359.7 - 323\right)\right) + 22.56\left(31.1\left(2359.7 - 323\right)\right)$$

$$\Rightarrow Q_H = 2514\ kJ$$

Since we calculated the first law efficiency of the steam cycle, we have:

$$W_{ideal} = \eta_{steam\_cycle} \cdot Q_H = 1063\ kJ$$

The second law efficiency of the cycle is given as 60%. Therefore:

$$W_{actual} = 0.6 \times W_{ideal} = 637.8\ \text{kJ}$$

Thus, the actual work produced by the system is 637.8 kJ per mole of biomass.

**d) What is the overall fuel utilization efficiency of this configuration? [5 points]**

The overall fuel utilization efficiency of the configuration can be calculated (per mole of biomass) as:

$$\eta_{conf} = \frac{W_{act}}{LHV_{C_6H_{12}O_6}} = \frac{637.8}{21000 \times 0.18} = 16.9\%$$

For Technology II: Gasification

e) What is the composition of the gas leaving the steam reformer if the temperature of the mixture is 500°C. Assume that this mixture of CO, CO2, H2 and H2O is at equilibrium. [10 points]
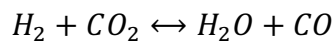
The reaction in the steam reformer has the following form:

$$C_6H_{12}O_6 + 6.5H_2O \rightarrow aCO + bH_2 + cH_2O + dCO_2$$
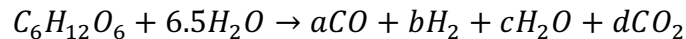
Mass balance for C, H, and O gives:

$$a + d = 6 \qquad b + c = 12.5 \qquad a + c + 2d = 12.5$$

We also the expression for product equilibrium:

$$H_2 + CO_2 \leftrightarrow H_2O + CO$$

At 500 C, K_p of the equilibrium is 0.24 (This can be determined by interpolating the K_p values (not $\log K_p$) using a polynomial expression of order 3 from the range 300 to 1200K. Therefore:

$$0.24 = \frac{ac}{bd}$$

Solving the four equations simultaneously, we have:

$$a = 2.555 \qquad b = 9.445 \qquad c = 3.055 \qquad d = 3.445$$

Therefore, the composition of the gas leaving the steam reformer (in terms of mole fractions) is:

$$X_{CO} = 0.138 \qquad X_{H_2} = 0.511 \qquad X_{H_2O} = 0.165 \qquad X_{CO_2} = 0.1862$$

f) What is the heat transfer required in the steam reformer? [7.5 points]

Writing the first law for the steam reformer, we have:

$$Q_{reform} = a\hat{h}_{CO,out} + b\hat{h}_{H_2,out} + c\hat{h}_{H_2O,out} + d\hat{h}_{CO_2,out} - \left(\hat{h}_{C_6H_{12}O_6,in} + 6.5\hat{h}_{H_2O,in}\right)$$

where for material i,

$$\hat{h}_i(T) = \hat{h}^o_{f,i} + \int_{T_o}^{T} \hat{c}_{p,i} dT$$

$$\hat{c}_{p,i} = a_i \Rightarrow \hat{h}_i(T) = \hat{h}^o_{f,i} + a_i(T - T_o)$$

and

$$T_{in} = 298\ K$$

$$T_{out} = 773\ K$$

We get the enthalpy values as:

$$\hat{h}_{C_6H_{12}O_6,in} = -1267.1\ kJ/mol$$

$$\hat{h}_{H_2O,in} = -286\ kJ/mol$$

$$\hat{h}_{CO,out} = -96.7\ kJ/mol$$

$$\hat{h}_{H_2,out} = 14.25\ kJ/mol$$

$$\hat{h}_{H_2O,out} = -223.9\ kJ/mol$$

$$\hat{h}_{CO_2,out} = -369.8\ kJ/mol$$

We already know the coefficient values. Therefore, we get:

$$Q_{reform} = 1055.65\ kJ$$

g) If CO concentration leaving the WGS is negligible, what is the hydrogen concentration in the gas leaving the WGS reactor? [7.5 points]

H_2O is added to match the moles of CO. We assume that the CO concentration leaving the WGS is negligible. Therefore, the WGS reaction has the form:

$$aCO + bH_2 + (a + c)H_2O + dCO_2 \rightarrow eH_2 + fCO_2 + gH_2O$$
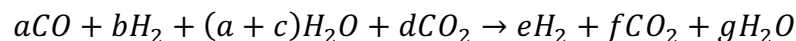
The atom balances are:

$$a + d = f \qquad a + b + c = g + e \qquad 2a + 2d + c = 2f + g$$

We can solve for the three unknowns to get:

$$e = 12 \qquad f = 6 \qquad g = 3.055$$

Therefore, the hydrogen concentration leaving the WGS reactor is:

$$X_{H_2} = \frac{12}{21.055} = 0.5699 = 56.99\%$$

h) **Evaluate the overall process efficiency, including the reforming and WGS process, if no waste heat is recuperated. [5 points]**

We can define the overall reformer efficiency as:

$$\frac{e \times LHV_{H_2}}{LHV_{C_6 H_{12} O_6} + Q_{reform}} = \frac{12 \times 242}{21000 \times 0.18 + 1055.65} = 0.6 = 60\%$$

2.60J Fundamentals of Advanced Energy Conversion
Spring 2020