

2.62 – Advanced Energy Conversion | Spring 2020

Homework 3 – Solutions

Problem 1

- a) How much heat is needed to pyrolyze the ammonia? [5 points]

First, we start by applying an enthalpy balance (first law), assuming we start from ambient conditions ($T_{in} = T_0 = 25\text{C}$):

$$Q = \sum_{prod} \nu_i h_i - \sum_{react} \nu_i h_i$$

$$Q = \left(0.5 \hat{c}_{p,N_2} (T_{out} - T_0) + 1.5 \hat{c}_{p,H_2} (T_{out} - T_0) \right) - \left(h_{f,NH_3}^o + \hat{c}_{p,NH_3} (T_{in} - T_0) \right)$$

$$Q = \left(0.5 \hat{c}_{p,N_2} (T_{out} - T_0) + 1.5 \hat{c}_{p,H_2} (T_{out} - T_0) \right) - (h_{f,NH_3}^o)$$

$$Q = (0.5 \times 29.15 \times (55) + 1.5 \times 28.96 \times (55)) - (-45,700 \text{ J}) = 48.89 \text{ kJ}$$

- b) Calculate the composition of the two streams at the exit of the cell.
[6 points | 8 points]

Begin by finding the inlet composition on the cathode side. Since the stoichiometry is 2:

$$\dot{n}_{O_2,c,in} = 2 \times \frac{\dot{n}_{H_2,c,in}}{2} = 1.5 \text{ mols/s}$$

$$\dot{n}_{N_2,c,in} = 3.76 \times \dot{n}_{O_2,c,in} = 5.64 \text{ mols/s}$$

The exit conditions on the cathode side are given by:

$$\dot{n}_{N_2,c,out} = \dot{n}_{N_2,c,in} = 5.64 \text{ mols/s}$$

$$\dot{n}_{O_2,c,out} = \dot{n}_{O_2,c,in} - \frac{\dot{n}_{H_2,a,consumed}}{2} = 1.5 - \frac{0.65 \times 1.5}{2} = 1.0125 \text{ mols/sec}$$

$$\dot{n}_{H_2O,c,out} = \dot{n}_{H_2,a,consumed} = 0.65 \times 1.5 = 0.975 \text{ mols/sec}$$

Likewise, the exit conditions on the anode side are given by:

$$\dot{n}_{N_2,a,out} = \dot{n}_{N_2,c,in} = 0.5 \text{ mols/s}$$

$$\dot{n}_{H_2,a,out} = (1 - 0.65) \times \dot{n}_{H_2,a,in} = 0.525 \text{ mols/s}$$

The corresponding exit mole fractions are summarized below:

	Cathode	Anode
H ₂	-	0.5122
O ₂	0.1327	-
N ₂	0.7394	0.4878
H ₂ O	0.1278	-

- c) Calculate the open circuit voltage of this cell based on the concentrations at the exit.
[6 points | 8 points]

To calculate the open circuit voltage, we use the Nernst Equation:

$$\begin{aligned} \Delta \mathcal{E}_{\max}(p^*, T^*) &= \Delta \mathcal{E}^o(T^*) - \frac{\sigma \mathcal{R}T^*}{n_e \mathcal{F}_a} \ln(p^*) - \frac{\mathcal{R}T^*}{n_e \mathcal{F}_a} \ln \left(\frac{\prod_{\text{prod}} X_i^{v_i''}}{\prod_{\text{react}} X_i^{v_i'}} \right) \\ &= \Delta \mathcal{E}^o(T^*) + \Delta \mathcal{E}_p(p^*, T^*) + \Delta \mathcal{E}_{\text{conc}}(X_i, T^*) \end{aligned}$$

The equilibrium constant K_p for the reaction $H_2 + 0.5O_2 \rightarrow H_2O$ at a standard pressure of 1 atm and at 80°C is calculated based on Table 3.6 in the notes. Using linear interpolation (note this is a simplification), $K_p = 10^{35.3259} = 2.118 \times 10^{35}$ (no units).

$$K_p(T) = \exp \left(\frac{-\Delta G^o(T)}{\mathcal{R}T} \right)$$

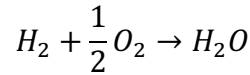
Therefore:

$$\Delta \mathcal{E}^o(T^*) = \frac{\mathcal{R}T^*}{n_e \mathcal{F}_a} \ln K_p(T^*) = \frac{(8.314 \times 353.15)}{(2 \times 96485.33)} \ln(2.118 \times 10^{35}) = 1.238 \text{ V}$$

Similarly:

$$\Delta \varepsilon_p(p^*, T^*) = -\frac{\sigma \mathcal{R} T^*}{n_e \mathfrak{S}_a} \ln\left(\frac{p^*}{p_0}\right) = \frac{0.5 \times (8.314 \times 353.15)}{(2 \times 96485.33)} \ln(2) = 0.00527 \text{ V}$$

Given the reaction in the cell:



The last term is calculated as:

$$\Delta \varepsilon_c(X_i, T^*) = -\frac{\mathcal{R} T^*}{n_e \mathfrak{S}_a} \ln\left(\frac{\prod_{prod} X_i^{v_i''}}{\prod_{react} X_i^{v_i'}}\right) = \frac{(8.314 \times 353.15)}{(2 \times 96485.33)} \ln\left(\frac{X_{H_2, anode} X_{O_2, cathode}^{1/2}}{X_{H_2O, cathode}}\right)$$

$$\Delta \varepsilon_c(X_i, T^*) = 0.00576 \text{ V}$$

Summing up all components:

$$\Delta \varepsilon_{max}(p^*, T^*) = 1.25 \text{ V}$$

- d) Calculate the power delivered by the stack of 200 cells in the proposed application. [2.5 points]**

$$P = j \times A \times V \times n = 600 \frac{\text{mA}}{\text{cm}^2} \times 2000 \text{ cm}^2 \times 0.65 \text{ V} \times 200 = 156 \text{ kW}$$

- e) What is the mass flow rate of H₂ needed to generate the power? [4 points | 5 points]**

To supply a current of $I = 1200$ Amps, the number of moles of electrons needed per second is $N_e = I/F$ (where F is the Faraday number). Since each mole of H₂ supplies $n_e = 2$ moles of electrons, we get:

$$\dot{n}_{H_2} = \frac{I}{n_e F} = \frac{1,200}{2 \times 96485.33} = 0.00622 \text{ mols/s}$$

For a stack of 200 cells, we will need:

$$\dot{n}_{H_2, consumed} = 200 \times 0.00622 = 1.244 \text{ mols/s}$$

However, only 65% of H₂ is consumed (react and contribute electrons to the current) (see Figure 1). Thus, the total mole flowrate of H₂ needed is:

$$\dot{n}_{H_2, supplied} = \frac{1.244 \text{ mols/s}}{0.65} = 1.914 \text{ mols/s}$$

Assuming a molar mass of 2g/mole for H₂, this translates to a H₂ mass flowrate of **3.828 grams/sec**.

- f) **What is the cooling rate required to keep the fuel cell at the desired temperature?**
Note that the inlet and exit streams are all at the same temperature as the cell.
[4 points | 5 points]

Assuming steady state, and ignoring kinetic and potential energy changes, we get the following equation by conserving energy around the fuel cell (the control volume is specified in the figure below). Here $\dot{Q}_{cooling}$ is positive according to the arrow shown in the figure.

$$\dot{Q}_{cooling} + \dot{W}_{elec} = \sum_{inlet} \dot{n}_i h_i - \sum_{outlet} \dot{n}_i h_i$$

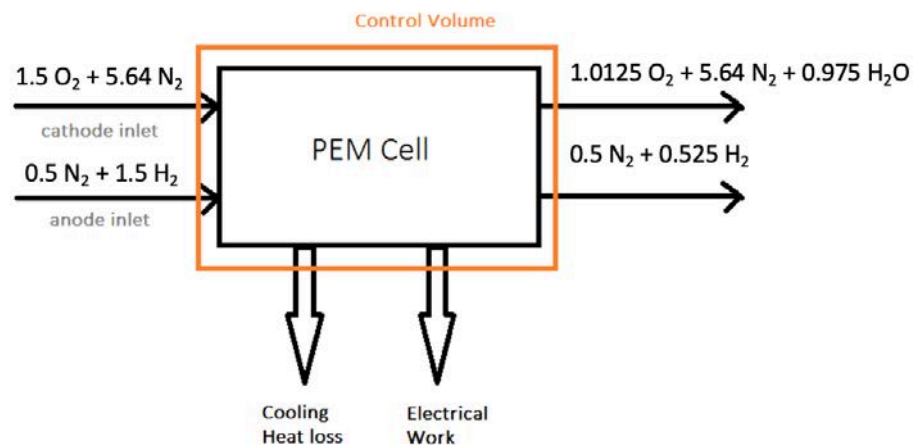


Figure 1 - Control volume to calculate cooling rate

$\dot{W}_{elec} = 156 \text{ kW}$ from part d. The right-hand side is essentially the heat released from the combustion of 1.244 moles of H₂ per second (the number of moles of H₂ participating in electrochemical reactions per second, as calculated in part e). This evaluates to $1.244 \times \text{LHV}_{H_2}$ and $\dot{Q}_{cooling} = 144.8 \text{ kW}$.

g) What is the efficiency of the cell? [2.5 points | 3.5 points]

We use the HHV value for H₂ (since water will be leaving in liquid phase under the specified conditions) and rate of fuel consumed to be more reasonable in the analysis:

$$\eta_{FU} = \frac{\text{Power Out}}{\text{Rate of Chemical Energy In}} = \frac{IV_{act}}{\dot{n}_f \Delta \hat{h}_{R,c}^\circ} = \frac{156000}{(1.244 \times 285800)} = 43.9\%$$

h) Is it better efficiency-wise to operate the cell at 10 atm? [8 points]

If the fuel cell were operated at 10 atm, the open circuit voltage would be increased by:

$$\begin{aligned} \Delta \varepsilon_{p,2}^\circ(p^*, T^*) - \Delta \varepsilon_{p,1}^\circ(p^*, T^*) &= -\frac{\sigma \mathcal{R} T^*}{n_e \mathfrak{S}_a} \ln\left(\frac{p_2^*}{p_1^*}\right) = \frac{0.5 \times (8.314 \times 353.15)}{(2 \times 96485.33)} \ln\left(\frac{10}{2}\right) \\ &= 0.0122 \text{ V} \end{aligned}$$

Therefore, for every 1.5 moles of hydrogen supplied (see Figure 1), we get an additional electric work of $\delta \dot{w} = 1.5 n_e F (d\Delta \varepsilon) = 3,531.4 \text{ W}$.

Corresponding to 1.5 moles of hydrogen supplied, 7.14 moles of air are supplied (see Figure 1). Thus, the compression work (for an ideal, isothermal compressor operating at $T = 80^\circ\text{C} = 353.15 \text{ K}$ and a pressure ratio of 5) is:

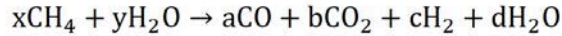
$$\dot{w}_{comp} = \dot{n} R T \ln\left(\frac{p_2^*}{p_1^*}\right) = 7.14 \times 8.314 \times 353.15 \times \ln(5) = 33.74 \text{ kW}$$

Stated differently, we are getting an addition 3.5 kW electric power by supplying 33.74 kW mechanical power to the compressor, which is not desirable.

Problem 2

- a) Determine the molar flow rate of methane and water fed to the reformer. Note that the partial pressure-based equilibrium constant of the water gas shift reaction at 800 C is $K_p = 0.8879$. [7 points | 10 points]

Across the reformer/water gas shift reactor, we can write a chemical reaction equation as,



From the given molar conditions,

$$b = 0.049$$

$$d = 0.284$$

Water gas shift reaction is



Using the thermodynamic equilibrium constant,

$$K_p = \frac{\left(\frac{P_{\text{CO}_2}}{P_0}\right)\left(\frac{P_{\text{H}_2}}{P_0}\right)}{\left(\frac{P_{\text{CO}}}{P_0}\right)\left(\frac{P_{\text{H}_2\text{O}}}{P_0}\right)} = \frac{bc}{ad} = \frac{0.049c}{0.284a} = 0.8879$$

It gives,

$$a = 0.1943c \quad (1)$$

Mass balance gives,

$$\text{C balance: } x = a + b = a + 0.049 \quad (2)$$

$$\text{H balance: } 4x + 2y = 2c + 2d = 2c + 2 \times 0.284 = 2c + 0.568 \quad (3)$$

$$\text{O balance: } y = a + 2b + d = a + 2 \times 0.049 + 0.284 = a + 0.382 \quad (4)$$

We have 4 equations (1 - 4) and 4 unknowns (a, c, x, and y). Combining 4 equations,

$$\begin{aligned} 4x + 2y &= 4(a + 0.049) + 2(a + 0.382) = 6a + 0.96 = 2c + 0.568 \\ 6(0.1943)c + 0.96 &= 2c + 0.568 \end{aligned}$$

Thus,

$$a = 0.0913, \quad c = 0.47, \quad x = 0.1403, \quad y = 0.4733$$

Therefore,

$$\begin{aligned} \text{CH}_4 &: 0.1403 \text{ kmol/s} \\ \text{H}_2\text{O} &: 0.4733 \text{ kmol/s (Ans)} \end{aligned}$$

- b) Calculate the flow rate of hydrogen and the current produced by the fuel cell. [3 points | 5 points]

From the answer to the question 1,

$$\dot{n}_{\text{H}_2} = c = 0.47 \text{ kmol/s (Ans)}$$

Using the faraday constant F_a ,

$$I = n_e F_a \dot{n}_{\text{H}_2} = 2 \times 96485 \times 0.47 \times 1000 = 90.7 \times 10^6 \text{ A (Ans)}$$

- c) Determine the heat transfer rate across the reformer/water gas shift reactor. [5 points | 7.5 points]

Applying the first law to the reformer/water gas shift reactor,

$$0 = \dot{Q}_1 - \dot{W}_{\text{out}} + \sum_{\text{in}} \dot{n}_{\text{in}} \hat{h}_{\text{in}} - \sum_{\text{out}} \dot{n}_{\text{out}} \hat{h}_{\text{out}}$$

Across the reformer/water gas shift reactor, $\dot{W}_{\text{out}} = 0$. Thus,

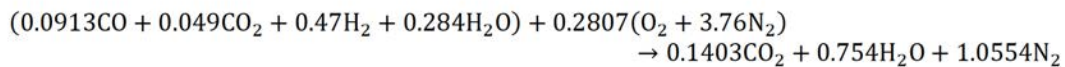
$$\begin{aligned} \dot{Q}_1 &= \sum_{\text{out}} \dot{n}_{\text{out}} \hat{h}_{\text{out}} - \sum_{\text{in}} \dot{n}_{\text{in}} \hat{h}_{\text{in}} \\ &= [\dot{n}_{\text{CO}} \hat{h}_{\text{CO}} + \dot{n}_{\text{CO}_2} \hat{h}_{\text{CO}_2} + \dot{n}_{\text{H}_2} \hat{h}_{\text{H}_2} + \dot{n}_{\text{H}_2\text{O}} \hat{h}_{\text{H}_2\text{O}}] - [\dot{n}_{\text{CH}_4} \hat{h}_{\text{CH}_4} + \dot{n}_{\text{H}_2\text{O}} \hat{h}_{\text{H}_2\text{O}}] \\ &= [0.0913 \times (-86410) + 0.049 \times (-356100) + 0.47 \times (22900) + 0.284 \times (-212800)] \\ &\quad - [0.1403 \times (-74610) + 0.4733 \times (-285900)] \\ &= 70772 \text{ kJ/s} \end{aligned}$$

Therefore,

$$\dot{Q}_1 = 70772 \text{ kJ/s (Ans)}$$

- d) Calculate the flow rate of air into the fuel cell. [5 points | 7.5 points]

Because the stream (1)/air ratio is stoichiometric,



Thus,

$$\dot{n}_{\text{air}} = 0.2807(1 + 3.76) = 1.336 \text{ kmol/s (Ans)}$$

- e) Assuming that the product stream (2) of the fuel cell consists of CO, CO₂, and H₂O, determine the maximum work transfer of the fuel cell. [6 points | 10 points]

Because only hydrogen reacts as a fuel and the fuel utilization is 100%,

$$\begin{aligned} & \left(\begin{array}{c} (0.0913\text{CO} + 0.049\text{CO}_2 + \mathbf{0.47}\mathbf{H}_2 + 0.284\text{H}_2\text{O}) \\ \text{anode inlet} \end{array} \right) + \left(\begin{array}{c} (\mathbf{0.235}\mathbf{O}_2 + 0.0457\text{O}_2 + 1.0554\text{N}_2) \\ \text{cathode inlet} \end{array} \right) \\ & \rightarrow \left(\begin{array}{c} (0.0913\text{CO} + 0.049\text{CO}_2 + \mathbf{0.47}\mathbf{H}_2\mathbf{O} + 0.284\text{H}_2\text{O}) \\ \text{anode outlet} \end{array} \right) + \left(\begin{array}{c} (0.0457\text{O}_2 + 1.0554\text{N}_2) \\ \text{cathode outlet} \end{array} \right) \end{aligned}$$

To get the maximum work transfer, we need to calculate the negative of the change in Gibbs free energy for the given temperature and the pressure. Thus,

$$\begin{aligned} \dot{W}_{\max} &= -\Delta G_{\text{rxn}}(T, p) = -\Delta G_{\text{rxn}}^{\circ}(T) - \sigma \bar{R}T \ln \left(\frac{P}{P_0} \right) - \bar{R}T \ln \left(\frac{\prod_{\text{prod}} X_i^{v''_i}}{\prod_{\text{react}} X_i^{v''_i}} \right) \\ \dot{W}_{\max} &= -\Delta G_{\text{rxn}}^{\circ}(T = 800\text{C}) - \sigma \bar{R}T \ln \left(\frac{P}{P_0} \right) \\ &\quad - \bar{R}T \left(\dot{n}_{\text{H}_2\text{O}, a, \text{out}} \ln X_{\text{H}_2\text{O}, a, \text{out}} + \dot{n}_{\text{O}_2, c, \text{out}} \ln X_{\text{O}_2, c, \text{out}} + \dot{n}_{\text{N}_2, c, \text{out}} \ln X_{\text{N}_2, c, \text{out}} - \dot{n}_{\text{H}_2, a, \text{in}} \ln X_{\text{H}_2, a, \text{in}} + \dot{n}_{\text{O}_2, c, \text{in}} \ln X_{\text{O}_2, c, \text{in}} + \dot{n}_{\text{N}_2, c, \text{in}} \ln X_{\text{N}_2, c, \text{in}} \right) \\ &= 88595 + 4827 - 5977 \\ &= 87445 \text{ kJ/s} \end{aligned}$$

The CO₂ and CO terms cancel out as the total molar flow rate at the anode is constant.

- f) Determine the actual work transfer from the fuel cell, assuming a second law efficiency of 70% for the fuel cell. [2 points | 2.5 points]

$$\dot{W}_1 = \dot{W}_{\max} \times \eta_{\text{II}} = 87445 \times 0.7 = 61211 \text{ kJ/s (Ans)}$$

- g) Calculate the operating voltage of the fuel cell. [2 points | 2.5 points]

Based on the power output \dot{W}_1 ,

$$V = \frac{\dot{W}_1}{I} = \frac{61211 \times 1000}{90.7 \times 10^6} = 0.675 \text{ V (Ans)}$$

Problem 3

- a) Determine the mole fractions at the anode and cathode. What is the theoretical open circuit voltage of this cell? [12 points]

Anode:

Start by using the information we have for water vapor:

$$\phi_{in} = \frac{P_v}{P_{sat}} = \frac{X_v P_0}{P_{sat}} \quad \rightarrow \quad X_{H_2O} = \phi_{in} \left(\frac{P_{sat}}{P_0} \right) = 0.2 \times 0.4708 = 0.09416$$

Given the molar ratio of H₂ to CO₂:

$$X_{H_2} = (1 - X_{H_2O}) \times \frac{4}{5} = 0.7247$$

$$X_{CO_2} = (1 - X_{H_2O}) \times \frac{1}{5} = 0.1812$$

Cathode:

Start by using the information we have for water vapor:

$$\phi_{in} = \frac{P_v}{P_{sat}} = \frac{X_v P_0}{P_{sat}} \quad \rightarrow \quad X_{H_2O} = \phi_{in} \left(\frac{P_{sat}}{P_0} \right) = 0.4 \times 0.4708 = 0.18832$$

Given the molar ratio of N₂ to O₂:

$$X_{O_2} = (1 - X_{H_2O}) \times \frac{1}{4.76} = 0.1705$$

$$X_{N_2} = (1 - X_{H_2O}) \times \frac{3.76}{4.76} = 0.6412$$

Theoretical Open Circuit Voltage:

We do this calculation based on inlet conditions – assuming each stream is pure:

Taking $T_0 = 298 \text{ K}$, the properties @ (353K and 1) bar are calculated as follows:

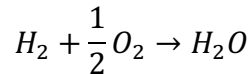
$$h_i = \hat{c}_p(T_i - T_0) + h_{f,i}^o$$

$$s_i = s_i^o + \hat{c}_p \ln\left(\frac{T_i}{T_0}\right)$$

$$g_i = h_i - T_i s_i$$

	Enthalpy (J/mol)	Entropy (J/mol-K)	Gibbs free energy (J/mol)
H2	1592.8	135.5851	-46268.8
O2	1625.25	210.157	-72560.2
H2O	-239978.55	194.5243	-308645.6

In this case, the reaction occurring within the fuel cell is:



$$\Delta \varepsilon_{OC} = \frac{-\Delta G_R^o(353K)}{2F} + \frac{RT}{2F} \ln\left(\frac{X_{H_2,anode} X_{O_2,cathode}^{1/2}}{X_{H_2O,cathode}}\right) = 1.178 \text{ V}$$

- b) Determine What is the open circuit (thermodynamic) efficiency based on the lower heating value of H2? (LHV of H2 is 120.1 MJ/kg) [2 points]**

$$\Delta H_{LHV} = (120.1 \text{ MJ/kg}) \times (2.016 \text{ kg/kmol}) = 242,121.6 \text{ J/mol}$$

$$\eta_{OC} = \frac{\Delta G_R}{\Delta H_{LHV}} = \frac{2F(\Delta \varepsilon_{OC})}{\Delta H_{LHV}} = 93.9\%$$

- c) How many individual cells are needed to supply the required power for the vehicle? [2 points]**

$$Power = N_{cell} jVA$$

$$N_{cell} = \frac{Power}{jVA} = \frac{80,000 \text{ W}}{1 \frac{\text{A}}{\text{cm}^2} \times 0.6 \text{ V} \times 650 \text{ cm}^2} = 205 \text{ cells}$$

d) What is the total molar flow rate of oxygen? [2 points]

$$I = n_e F n_{O_2,consumed} = \frac{Power}{V}$$
$$\dot{n}_{O_2,consumed} = \frac{Power}{V(n_e F)} = \frac{80,000 \text{ W}}{4 \times 0.6 \text{ V} \times 96485 \text{ C/mol}} = 0.3455 \text{ mol/s}$$

Given the air stoichiometry is 2:

$$\dot{n}_{O_2,inlet} = 2 \times 0.3455 = 0.69 \text{ mol/s}$$

The corresponding molar flow rates of N₂ and H₂O at the inlet are:

$$\dot{n}_{N_2,in} = 3.76 \times \dot{n}_{O_2,inlet} = 2.59 \text{ mol/s}$$

$$\frac{\dot{n}_{H_2O,in}}{\dot{n}_{O_2,in}} = \frac{X_{H_2O,in}}{X_{O_2,in}} \rightarrow \dot{n}_{H_2O,in} = \left(\frac{0.18832}{0.1705} \right) \times 0.69 = 0.762 \text{ mol/s}$$

e) What is the composition of the air-side stream at the exit of the stack, expressed in terms of the mole fractions of N₂, O₂, and H₂O? [5 points]

$$\dot{n}_{H_2O,prod} = 2\dot{n}_{O_2,consumed} = 0.69 \text{ mol/s}$$

$$\dot{n}_{H_2O,exit} = \dot{n}_{H_2O,inlet} + \dot{n}_{H_2O,prod} = 1.452 \text{ mol/s}$$

$$\dot{n}_{O_2,exit} = \dot{n}_{O_2,inlet} - \dot{n}_{O_2,consumed} = 0.3445 \text{ mol/s}$$

$$\dot{n}_{N_2,exit} = \dot{n}_{N_2,inlet} = 2.59 \text{ mol/s}$$

Therefore:

$$X_{H_2O} = \frac{\dot{n}_{H_2O,exit}}{\dot{n}_{H_2O,exit} + \dot{n}_{O_2,exit} + \dot{n}_{N_2,exit}} = 0.331$$

$$X_{O_2} = \frac{\dot{n}_{O_2,exit}}{\dot{n}_{H_2O,exit} + \dot{n}_{O_2,exit} + \dot{n}_{N_2,exit}} = 0.0785$$

$$X_{N_2} = \frac{\dot{n}_{N_2,exit}}{\dot{n}_{H_2O,exit} + \dot{n}_{O_2,exit} + \dot{n}_{N_2,exit}} = 0.591$$

- f) When the design exit air relative humidity is 90%, does the current operating conditions satisfy the design target? [2 points]

$$\phi = \frac{P_{H_2O}}{P_{H_2O,sat}} = \frac{0.331}{0.4708} = 70\%$$

Therefore, the relative humidity is lower than the design target.

- g) What is the composition at the anode side exit stream? [6 points]

The molar fraction is independent of the total number of moles (provided the composition remains constant). Take the composition to be that of the anode inlet (Part a) such that $\sum n_i = 1$ mols of mixture (at anode inlet), and account for changes. Given the fuel utilization, we know that:

$$\phi = \frac{\dot{n}_{H_2,inlet} - \dot{n}_{H_2,exit}}{\dot{n}_{H_2,inlet}} = 0.9$$

$$\dot{n}_{H_2,exit} = 0.1\dot{n}_{H_2,inlet}$$

Similarly by mass conservation in the anode:

$$\dot{n}_{H_2O,exit} = \dot{n}_{H_2O,inlet} = \frac{X_{H_2O}}{X_{H_2}} \dot{n}_{H_2,inlet}$$

$$\dot{n}_{CO_2,exit} = \dot{n}_{CO_2,inlet} = \frac{X_{CO_2}}{X_{H_2}} \dot{n}_{H_2,inlet}$$

By the definition of molar fraction:

$$X_{H_2} = \frac{\dot{n}_{H_2,exit}}{\dot{n}_{H_2,exit} + \dot{n}_{CO_2,exit} + \dot{n}_{H_2O,exit}} = \frac{0.07247}{0.07247 + 0.1812 + 0.09416} = 0.208$$

$$X_{CO_2} = \frac{\dot{n}_{CO_2,exit}}{\dot{n}_{H_2,exit} + \dot{n}_{CO_2,exit} + \dot{n}_{H_2O,exit}} = \frac{0.1812}{0.07247 + 0.1812 + 0.09416} = 0.521$$

$$X_{H_2O} = \frac{\dot{n}_{H_2O,exit}}{\dot{n}_{H_2,exit} + \dot{n}_{CO_2,exit} + \dot{n}_{H_2O,exit}} = \frac{0.09416}{0.07247 + 0.1812 + 0.09416} = 0.271$$

h) What is the molar flow rate of the fuel stream at the inlet? [3 points]

$$I = n_e F n_{H_2,consumed} = \frac{Power}{V}$$

$$\dot{n}_{H_2,consumed} = \frac{Power}{V(n_e F)} = \frac{80,000 \text{ W}}{2 \times 0.6 \text{ V} \times 96485 \text{ C/mol}} = 0.691 \text{ mol/s}$$

Accounting for fuel utilization:

$$\dot{n}_{H_2,inlet} = \frac{\dot{n}_{H_2,consumed}}{0.9} = 0.7678 \text{ mol/s}$$

i) What is the first law efficiency of the cell? [2 points]

$$\eta_I = \frac{\text{generated power}}{\text{chemical energy in}} = \frac{80 \text{ kW}}{LHV_{H_2} \times \dot{n}_{H_2,inlet}} = \frac{80}{240.2 \times 0.7678} = 43.37\%$$

j) What is the cooling rate required to keep the fuel cell at 80C? [4 points]

$$0 = \sum_{in} \dot{n}_i h_i - \sum_{out} \dot{n}_i h_i + \dot{Q} - \dot{W}$$

$$\dot{Q} = \dot{W} + \sum_{out} \dot{n}_i h_i - \sum_{in} \dot{n}_i h_i$$

$$\dot{Q} = \dot{W} + (\dot{n}_{H_2O,produced} h_{H_2O}) - (\dot{n}_{H_2,consumed} h_{H_2}) - (\dot{n}_{O_2,consumed} h_{O_2})$$

$$\dot{Q} = 80 + 0.691 \times (-239.98) - (0.691 \times 1.59) - (0.3455 \times 1.63) = -87.49 \text{ kW}$$

k) Derive an expression for the exit relative humidity: [15 points]

By definition:

$$\phi_{exit} = \frac{\dot{n}_{H_2O,exit}}{\dot{n}_{H_2O,exit} + \dot{n}_{N_2,exit} + \dot{n}_{O_2,exit}} \frac{p^0}{P_{H_2O,sat}}$$

Expanding the terms:

$$\dot{n}_{O_2,consumed} = \frac{Power}{4VF}$$

$$\dot{n}_{N_2,exit} = \dot{n}_{N_2,inlet} = 3.76\lambda\dot{n}_{O_2,consumed}$$

$$\dot{n}_{O_2,exit} = \dot{n}_{O_2,inlet} - \dot{n}_{O_2,consumed} = (\lambda - 1)\dot{n}_{O_2,consumed}$$

To find the last term, we start by defining a ratio of vapor pressures:

$$\psi = \left(\frac{P_{H_2O,in}}{P_{N_2+O_2,in}} \right) = \left(\frac{\phi_{in} P_{H_2O,sat}}{P_0 - \phi_{in} P_{H_2O,sat}} \right)$$

Likewise, using the definition of partial pressure:

$$\psi = \left(\frac{X_{H_2O,in}}{X_{N_2+O_2,in}} \right) = \left(\frac{n_{H_2O,in}}{n_{N_2+O_2,in}} \right)$$

For one mole of oxygen entering, this becomes:

$$\psi = \left(\frac{n_{H_2O,in}}{4.76} \right) \rightarrow n_{H_2O,in} = 4.76\psi \text{ (per mole of } O_2)$$

Accounting for the total amount of oxygen entering:

$$\dot{n}_{H_2O,in} = 4.76\lambda\psi\dot{n}_{O_2,consumed}$$

Also we know that:

$$\dot{n}_{H_2O,produced} = 2\dot{n}_{O_2,consumed}$$

Therefore:

$$\dot{n}_{H_2O,exit} = \dot{n}_{H_2O,inlet} + \dot{n}_{H_2O,produced} = 4.76\lambda\psi\dot{n}_{O_2,consumed} + 2\dot{n}_{O_2,consumed}$$

Substituting back into our starting equation:

$$\begin{aligned}\phi_{exit} &= \frac{\dot{n}_{H_2O,exit}}{\dot{n}_{H_2O,exit} + \dot{n}_{N_2,exit} + \dot{n}_{O_2,exit}} \frac{p^0}{p_{H_2O,sat}} \\ \phi_{exit} &= \frac{4.76\lambda\psi + 2}{4.76\lambda\psi + 2 + 3.76\lambda + (\lambda - 1)} \frac{p^0}{p_{H_2O,sat}} \\ &= \frac{4.76\lambda\psi + 2}{4.76\lambda\psi + 4.76\lambda + 1} \frac{p^0}{p_{H_2O,sat}} = \frac{\lambda\psi + 0.42}{\lambda(\psi + 1) + 0.21} \frac{p^0}{p_{H_2O,sat}}\end{aligned}$$

- 1) What should be the relative humidity of the inlet air if the relative humidity of the exit air is 90%? [5 points]**

We start by solving for the ratio of vapor pressures:

$$\phi_{exit} = 0.9 = \frac{2\psi + 0.42}{2\psi + 2.21} \frac{1}{0.4708}$$

$$\psi = \frac{\phi_{inlet} p_{H_2O,sat}}{p^0 - \phi_{inlet} p_{H_2O,sat}} = 0.448$$

Using the definition of the ψ :

$$\frac{1}{\psi} = \frac{p^0 - \phi_{inlet} p_{H_2O,sat}}{\phi_{inlet} p_{H_2O,sat}} = \frac{1}{\phi_{inlet} 0.4708} - 1 = \frac{1}{0.448}$$

$$\phi_{inlet} = 0.657$$

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Spring 2020

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