Homework 3

2.60/2.62/10.390 Fundamentals of Advanced Energy Conversion
Spring 2020

Total points: 100 (Undergraduate) | 150 (Graduate)

Problem 1. Proton Exchange Membrane (PEM) Fuel Cell [30% for Undergrads and Grads]

A PEM (Proton Exchange Membrane) fuel cell operates at 80°C and 2 atm. The fuel is a product of ammonia pyrolysis to N_2 and H_2. Air is the oxidizer, and the outlet stream consists of nitrogen, oxygen and water (reaction products) as shown in **Figure 1**. Only 65% of the fuel is used (and the rest is recycled). The air flow rate is such that, at the inlet, there is twice as much oxygen as needed to consume all the hydrogen.

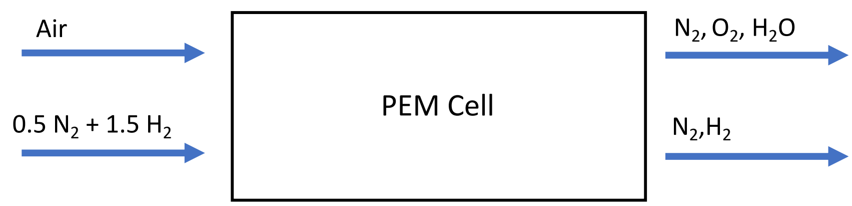

Figure 1 - PEM Fuel Cell

Consider this cell in operation, with a voltage of 0.65V and current density of 600 mA/cm². The effective total area of the cell is 2000 cm². A stack of 200 such cells is used in series for a stationary application (such that their voltages add up).

<u>Please answer the following:</u>

a. How much heat is needed to pyrolyze the ammonia?

b. Calculate the composition of the two streams at the exit of the cell.

c. Calculate the open circuit voltage of this cell based on the concentrations at the exit.

d. Calculate the power delivered by the stack of 200 cells in the proposed application.

e. What is the mass flow rate of H_2 needed to generate the power?

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.

g. What is the efficiency of the cell?

h. **(For graduate students only)** If the cell is operating very close to open circuit conditions, is it better efficiency-wise to operate the cell at 10 atm? Assume that the input H_2-N_2 mixture is available at 1 atm, and an isothermal (and ideal) air compressor is available at 80°C.

Problem 2. Methane Fuel Cell System [30% for Undergrads and Grads]

A fuel cell system is proposed as shown in **Figure 2.** The system utilizes methane and air. All stream conditions are given in the figure. Across the fuel cell, assume that only hydrogen is consumed in the electrochemical reactions with 100% hydrogen utilization. Carbon monoxide passes through the fuel cell without change. Within the cell, O^{2-} ions move through the electrolyte from the cathode to the anode. The flow rate of air at the cathode inlet is determined such that the ratio of the flow rate of the fuel stream (1) to the air stream is stoichiometric. All gases can be treated as ideal gases.

Assume that stream (1) at the exit of the reformer/water gas shift reactor consists of CO, CO_2, H_2 and H_2O. The products are at thermodynamic equilibrium at the given temperature and pressure. At equilibrium, there are 0.049 kmol/s of CO_2 and 0.284 kmol/s of H_2O within the product stream (1).

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.

b. Calculate the flow rate of hydrogen and the current produced by the fuel cell.

c. Determine the heat transfer rate across the reformer/water gas shift reactor.

d. Calculate the flow rate of air into the fuel cell.

e. Assuming that the product stream (2) of the fuel cell consists of CO, CO_2, and H_2O, determine the maximum work transfer of the fuel cell.

f. Determine the actual work transfer from the fuel cell, assuming a second law efficiency of 70% for the fuel cell.

g. Calculate the operating voltage of the fuel cell.

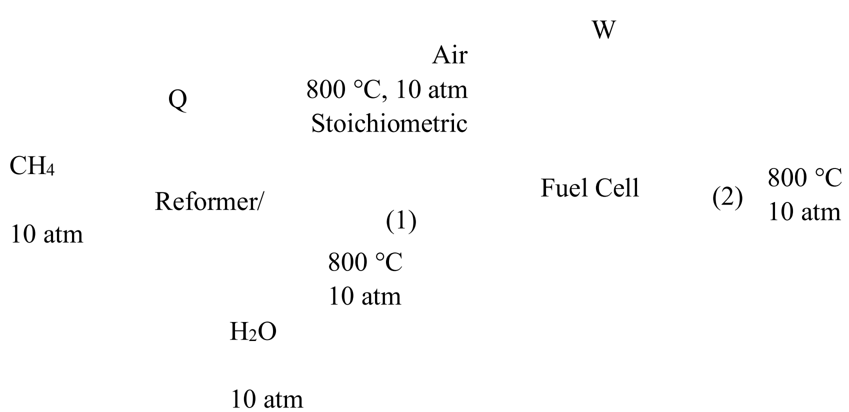

Figure 2 - Methane Fuel Cell System

Problem 3. PEMFC & Water Management [40% for Undergrads and Grads]

Water management is critical for the operation of proton exchange membrane fuel cells (PEMFC). These cells use sulphonate fluoropolymers as an electrolyte (membrane). The most well-known membrane brand is Nafion. For the electrolyte to be a good proton conductor, it should be well hydrated. However, too much water can flood the electrodes blocking gas diffusion through the pores. Therefore, water produced by the electrochemical reaction on the cathode side should be removed by airflow. Even though both the fuel and air streams are mixed with water vapor at the inlet, humidity level is controlled primarily by air stream.

The following figure shows a schematic diagram for the operation of a fuel cell operating on hydrogen produced by steam reforming of methane.

$H_2 + CO_2 + H_2O$

T = 80 ˚C

Air + H_2O

Figure 3 - Proton Exchange Membrane Fuel Cell Setup

We will make following assumptions:

- All streams are at 1 bar and 80C.
- The fuel consists of H_2 and CO_2 with a molar ratio 4:1. The relative humidity of fuel steam is 20%, where the relative humidity is defined as:

$$\phi = \frac{p_{H_2O}}{p_{H_2O,sat}(T)}$$

- CO, which is poisonous to Pt catalyst, is completely removed from the fuel stream.
- Air stoichiometry, defined as the ratio of inlet oxygen flow rate to the oxygen consumption rate is 2 at the inlet, a very typical value.

$$\lambda = \frac{\dot{n}_{O_2,inlet}}{\dot{n}_{O_2,usage}}$$

- The inlet air relative humidity is 40%.
- The electrolyte is well hydrated and the level of hydration is constant and steady. In other words, there is no incoming and outgoing water from and to the electrolyte.
- Water produced electrochemically is in the form of vapor.
- All the species are considered as an ideal gas
- Values given at 353K, saturated steam pressure: 0.4708×10^5 Pa:

c_p (Temp range [298K~353K])	Enthalpy of formation (J/ mol)	Entropy of formation (J/ mol-K) @ 1 bar
$\hat{c}^0_{p,O_2} = 29.55$ $\hat{c}^0_{p,H_2} = 28.96$ $\hat{c}^0_{p,H_2O} = 33.59$ $\hat{c}^0_{p,N_2} = 29.15$	$\hat{h}^0_{f,H_2O(g)} = -241,826$	$\hat{s}^0_{f,H_2O(g)} = 188.835$ $\hat{s}^0_{f,H_2} = 130.68$ $\hat{s}^0_{f,O_2} = 205.152$ $\hat{s}^0_{f,N_2} = 191.609$

Answer the following questions:

a. Determine the mole fractions at the anode and cathode. What is the theoretical open circuit voltage of this cell?
b. What is the open circuit (thermodynamic) efficiency based on the lower heating value of H_2? (LHV of H_2 is 120.1 MJ/kg)

A fuel cell stack is used to power a small vehicle that requires 80 kW. Each cell operates at 0.6V, and a typical current density is 1 A/cm^2. Assume that the surface area of each individual cell is 650 cm^2, the Faradaic efficiency is 100% and the fuel utilization is 90%.

c. How many individual cells are needed to supply the required power for the vehicle?
d. What is the total molar flow rate of oxygen?
e. What is the composition of the air-side stream at the exit of the stack, expressed in terms of the mole fractions of N_2, O_2, and H_2O?
f. When the design exit air relative humidity is 90%, does the current operating conditions satisfy the design target?
g. What is the composition at the anode side exit stream?
h. What is the molar flow rate of the fuel stream at the inlet?
i. What is the first law efficiency of the cell?

$$\eta_I = \frac{generated\ power}{rate\ of\ chemical\ energy\ in}$$

j. What is the cooling rate required to keep the fuel cell at 80C?
k. **(Graduate students only)** Derive an expression for the exit relative humidity in terms of the air stoichiometry, λ , the relative humidity of the inlet air stream, ϕ_{inlet}, the water saturation pressure, $p_{H_2O,sat}$, and the pressure p^0.
l. **(Graduate students only)** What should be the relative humidity of the inlet air if the relative humidity of the exit air is 90%?