## 2.62 – Advanced Energy Conversion | Spring 2020

## **Homework 4 – Solutions**

### Problem 1 (35%)

a) Drive a relation between the open circuit potential of the cell and the oxygen concentration in the products stream. Plot this relation when the cell temperature is 25 C, 100 C and 400 C? [15 points]

First, we use the Nernst Equation for the reaction noting that no reaction occurs:

$$\chi_{react} = \chi_{prod}$$

$$\Delta \mathcal{E}_{\max}(p^*, T^*) = \Delta \mathcal{E}^o(T^*) - \frac{\sigma \Re T^*}{n_e \Im_a} \ell n(p^*) - \frac{\Re T^*}{n_e \Im_a} \ell n\left( \frac{\prod_{prod} X_i^{v_i^*}}{\prod_{react} X_i^{v_i^*}} \right) \\ = \Delta \mathcal{E}^o(T^*) + \Delta \mathcal{E}_p(p^*, T^*) + \Delta \mathcal{E}_{conc}(X_i, T^*)$$

Simplifying the equation yields (in terms of the partial pressures):

$$\Delta \varepsilon = -\frac{RT}{n_e \Im_a} \ln\left(\frac{p_{\chi}'}{p_{\chi}'}\right)$$

Noting that we have oxygen on both sides and given the oxygen concentration in air:

$$\Delta \varepsilon = -\frac{RT}{n_e \mathfrak{I}_a} \ln\left(\frac{p_{O_2}''}{p_{O_2}'}\right) = -\frac{RT}{n_e \mathfrak{I}_a} \ln\left(\frac{p_{O_2}''}{0.21}\right) = -\frac{RT}{n_e \mathfrak{I}_a} \ln\left(\frac{X_{O_2}''}{0.21}\right)$$

Plotting this relationship for the temperatures indicated:

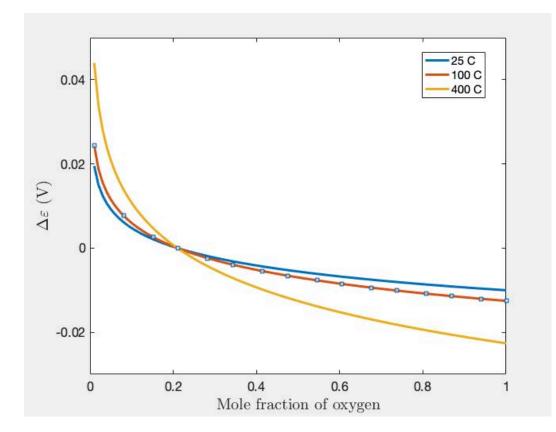


Figure 1 - Open circuit potential as a function of oxygen concentrations in the products stream

Note for one mole of oxygen, 4 moles of electrons are generated ( $n_e = 4$ ). As can be seen, the voltage drops as a function of molar concentration in the products stream. Note the crossover point that occurs at  $X''_{O_2} = 0.21$ . At that point, a reversal in the voltage sign occurs given the nature of the logarithmic relationship. An increase in temperature amplifies the voltage in either direction (positive or negative).

b) Drive an expression for the open circuit potential and the ideal work of expansion in this case in terms of the hydrogen partial pressure ratio across the electrolyte. Compare this expression with the isothermal mechanical work of expansion across the same pressure ratio. Comment on this result. Calculate the open circuit potential at T = 30 C, and hydrogen pressure ratio across the electrolyte of 100 and 10,000. [10 points]

For hydrogen, an expression similar to the one presented previously is obtained.

$$\Delta \varepsilon = -\frac{RT}{n_e \Im_a} \ln\left(\frac{p_{H_2}''}{p_{H_2}'}\right)$$

Noting that per molecule of hydrogen consumed two electrons are generated, the work may be expressed as:

$$W = 2\Im_a \Delta \varepsilon = -RT \ln \left( \frac{p_{H_2}''}{p_{H_2}'} \right)$$

Interestingly, we can show that this is the same result as applying the first and second laws of thermodynamics in isothermal expansion.

$$Q = W$$
$$Q = T\Delta S = RT \ln\left(\frac{p_2}{p_1}\right)$$

Calculating the open circuit potential for the conditions specified:

$$\Delta \varepsilon_1 = -\frac{RT}{n_e \mathfrak{I}_a} \ln\left(\frac{p_{H_2}''}{p_{H_2}'}\right) = -\frac{(8.314 \times 303.15)}{(2 \times 96485.33)} \ln(1/100) = 0.06 \text{ V}$$
$$\Delta \varepsilon_2 = -\frac{RT}{n_e \mathfrak{I}_a} \ln\left(\frac{p_{H_2}''}{p_{H_2}'}\right) = -\frac{(8.314 \times 303.15)}{(2 \times 96485.33)} \ln(1/10000) = 0.12 \text{ V}$$

c) Drive an expression for the efficiency of this cycle and compare it to that of a conventional Bryton cycle between the same two pressures. Calculate both efficiencies for pressure ratio of 30, T1 = 300 K and T3 = 1600 K. [10 points]

The T-s diagram comparing both cycles is shown Figure 2. In this figure, the proposed cycle is given by the states 1-2-3-4, whereas the Brayton cycle is given by the states 1-5-3-4. The efficiency of the Brayton cycle is given in terms of the pressure ratio  $\pi_p$  (refer Chapter 5 in the notes):

$$\eta_{Br} = 1 - \left(\frac{1}{\pi_p}\right)^{\frac{k-1}{k}}$$

For air with an isentropic index of k = 1.4, this evaluates to:

$$\eta_{Br} = 1 - \left(\frac{1}{\pi_p}\right)^{\frac{k-1}{k}} = 1 - \left(\frac{1}{30}\right)^{\frac{1.4-1}{1.4}} = 62.2\%$$

For the proposed cycle with isothermal compression, the work of the compression process is given from Part b as:

$$W_c = -RT \ln\left(\frac{P_2}{P_1}\right) = -8.314 \times 300 \times \ln 30 = -8,483.2 \text{ J/mol}$$

Similarly, the work of the turbine is given by (refer to Chapter 5):

$$W_T = \left(\frac{k}{k-1}\right) RT_3\left(1 - \left(\frac{1}{\pi_p}\right)^{\frac{k-1}{k}}\right) = \left(\frac{1.4}{0.4}\right) \times 8.314 \times 1600 \times \left(1 - \left(\frac{1}{30}\right)^{\frac{0.4}{1.4}}\right)$$

$$W_T = 28,940 \text{ J/mol}$$

Therefore, the efficiency of the proposed cycle with isothermal compression is given by:

$$\eta = \frac{W_T + W_c}{c_p (T_3 - T_2)} = \frac{20,456.8}{29.2 \times (1300)} = 53.89\%$$

The efficiency is <u>lower</u> for the isothermal cycle given heat transfer occurring across a considerable temperature gradient from state 2 to 3.

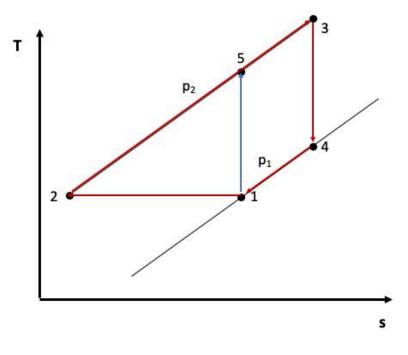
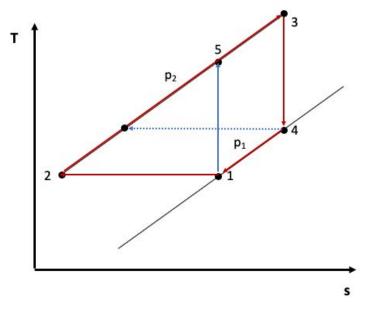


Figure 2 - T-s Diagram for the two cycles under consideration

# d) How can you improve the efficiency of the cycle proposed in (c) and what is the new efficiency? [10 points]

Noting the large input of heat necessary, the cycle may be improved by using regeneration to reduce  $Q_{in}$ . This is achieved by recovering the waste heat such that the lowest temperature in the cycle T<sub>4</sub>. This is illustrated in Figure 3, and the resulting efficiency is calculated as follows:

$$T_4 = T_3 \left(\frac{1}{\pi_p}\right)^{\frac{k-1}{k}} = 1600 \times \left(\frac{1}{30}\right)^{\frac{0.4}{1.4}} = 605.5 \text{ K}$$
$$\eta = \frac{W_T + W_c}{c_p(T_3 - T_4)} = \frac{20,456.8}{29.2 \times (994.5)} = 70\%$$



*Figure 3 - T-s diagram with improved cycle* 

e) Explain how the reverse of the set up described in part (b) can be used as an isothermal electrochemical compressor, in which a voltage is applied to pump the gas (hydrogen in the case of part (b)) from the low-pressure side to the high-pressure side. What is the open circuit voltage required to produce an oxygen stream at 10 bars from air? [7.5 points]

The application of a voltage reverses the driving force across the fuel cell such that hydrogen is transported from low pressure to high pressure and the cell effectively acts as an isothermal electrochemical compressor. The open circuit voltage necessary to produce an oxygen stream at 10 bars from air is given by:

$$\Delta \varepsilon = -\frac{RT}{n_e \Im_a} \ln\left(\frac{p_{O_2}''}{p_{O_2}'}\right) = -\frac{(8.314 \times 303.15)}{(4 \times 96485.33)} \ln\left(\frac{10}{0.21}\right) = -0.025 \text{ V}$$

### **Problem 2 (32.5%)**

# a) Determine the amount of steam injection and fuel consumption per unit mass of the air. [15 points Undergrad | 22.5 points Grad]

We start by fixing some of the states specified before proceeding. While state 1 is given, state 2 can be fixed by determining the temperature at the outlet of the compressor given the inlet conditions and the compression ratio. Hence, using the result from Chapter 5:

$$T_2 = T_1 \left( 1 + \frac{1}{\eta_c} \left[ \left( r_p \right)^{\frac{k-1}{k}} - 1 \right] \right) = 298 \left( 1 + \frac{1}{0.9} \left[ \left( 9 \right)^{\frac{1.39-1}{1.39}} - 1 \right] \right) = 580.2 \text{ K}$$

Similarly, for the turbine:

$$T_4 = T_3 \left( 1 - \eta_T \left[ 1 - \left( r_p \right)^{\frac{1-k}{k}} \right] \right) = 1423 \left( 1 - 0.85 \left[ 1 - (9)^{\frac{-0.29}{1.29}} \right] \right) = 951.53 \text{ K}$$

Furthermore, the conditions at the inlet and exit of the pump are defined using EES such that:

$$h_6 = 104.3 \text{ kJ/kg}$$
 and  $v_6 = 0.001 \text{ m}^3/\text{kg}$ 

As an incompressible fluid, the enthalpy at the pump exit is calculated as follows:

$$h_{7s} = h_6 + v(p_7 - p_6) = 104.3 + 0.001 \times (900 - 100) = 105.1 \text{ kJ/kg}$$

$$h_7 = h_6 + \frac{h_{7s} - h_6}{0.7} = 104.3 + \frac{0.8}{0.7} = 105.4 \text{ kJ/kg}$$

Next, we apply the first law across the combustor to arrive at the expression below. Note that the flow at the exit in state 3 is modeled as an ideal gas mixture of air + steam.

$$\sum_{reactants} H_i = \sum_{products} H_i$$

 $\dot{m}_{f,in}LHV_{f,in} + \dot{m}_{air,in}h_{air,in} + \dot{m}_{s,in}h_{s,in} = \dot{m}_{air,out}h_{air,out} + \dot{m}_{s,out}h_{s,out}$ 

 $\dot{m}_{f,in}LHV_{f,in} + \dot{m}_{air,2}h_{air,2} + \dot{m}_{s,8}h_{s,8} = \dot{m}_{air,3}h_{air,3} + \dot{m}_{s,3}h_{s,3}$ 

Dividing by the inlet air mass flow rate, using the hint provided, and applying mass balance:

$$\alpha \cdot LHV_{f,in} + h_{air,2} + \beta \cdot h_{s,8} = (1+\alpha)h_{air,3} + \beta h_{s,3}$$

where  $\alpha$  is the fuel-to-air mass ratio,  $\beta$  is the steam-to-air mass ratio.

Calculating the enthalpies using EES:

 $h_{air,2} = 586.6 \text{ kJ/kg}$ ,  $h_{air,3} = 1543 \text{ kJ/kg}$ ,  $h_{s,3} = 5021 \text{ kJ/kg}$ ,  $h_{s,8} = 3323 \text{ kJ/kg}$ 

Applying the first law to the HRSG, we arrive at the following:

$$\sum_{in} H_i = \sum_{out} H_i$$

$$\dot{m}_{air,4}h_{air,4} + \dot{m}_{s,4}h_{s,4} + \dot{m}_7h_7 = \dot{m}_{air,5}h_{air,5} + \dot{m}_{s,5}h_{s,5} + \dot{m}_8h_8$$

Diving by the inlet air mass flow rate and rearranging, we arrive at:

$$(1+\alpha)(h_{air,4} - h_{air,5}) + \beta(h_{s,4} - h_{s,5}) = \beta(h_8 - h_7)$$

The enthalpies are calculated to be:

$$h_{air,4} = 991.3 \text{ kJ/kg}$$
,  $h_{air,5} = 401.3 \text{ kJ/kg}$ ,  $h_{s,4} = 3880 \text{ kJ/kg}$ ,  
 $h_{s,5} = 2730 \text{ kJ/kg}$ 

Solving the enthalpy balance equations of the combustor and HRSG yield:

$$\alpha = 0.03$$
 and  $\beta = 0.2939$ 

#### b) Determine the net work produced by the cycle: [10.5 points Undergrad | 15.75 points Grad]

The net work produced by the cycle is given by:

$$W_{net} = W_T - W_c - W_p$$

where:

$$W_T = (1 + \alpha) (h_{air,3} - h_{air,4}) + \beta (h_{s,3} - h_{s,4}) = 903.7 \text{ kJ/kg}$$
$$W_c = h_2 - h_1 = 288.1 \text{ kJ/kg}$$
$$W_p = \beta (h_7 - h_6) = 0.3257 \text{ kJ/kg}$$

<u>Therefore:</u>

$$W_{net} = 903.7 - 288.1 - 0.3257 = 615.27 \text{ kJ/kg}$$

c) Determine the thermal efficiency of the cycle: [3.5 points Undergrad | 5.25 points Grad]

$$\eta_{th} = \frac{W_{net}}{\alpha \cdot LHV_f} = \frac{615.27}{0.03 \times 50050} = 40.98\%$$

d) Determine the simple gas turbine cycle efficiency (without the steam injection):[3.5 points Undergrad] 5.25 points Grad]

$$\eta = 1 - \left(\frac{1}{\pi_p}\right)^{\frac{k-1}{k}} = 1 - \left(\frac{1}{9}\right)^{\frac{0.34}{1.34}} = 42.7\%$$

### Problem 3 (32.5%)

a) Determine the amount of steam produced in the HRSG per unit mass of air. [12.5 points Undergrad | 18.75 points Grad]

We start by applying the first law to the HRSG:

$$\dot{m}_4(h_4 - h_5) = \dot{m}_7(h_8 - h_7)$$

Rearranging:

$$\alpha = \frac{h_4 - h_5}{h_8 - h_7}$$

We proceed to determining the enthalpies using EES and relationships from Chapter 5:

$$T_4 = T_3 \left( 1 - \eta_{GT} \left[ 1 - \left( r_p \right)^{\frac{1-k}{k}} \right] \right) = 1500 \times \left( 1 - 0.88 \left( 1 - 8^{-\frac{0.323}{1.323}} \right) \right) = 975.1 \text{ K}$$

$$h_4 = 1018 \text{ kJ/kg}$$
,  $h_5 = 424.6 \text{ kJ/kg}$ 

For state 6, the liquid water is a saturated liquid at  $P_6 = 6$  kPa:

$$h_6 = 151.5 \text{ kJ/kg}, v_6 = 0.001 \text{ m}^3/\text{kg}$$

Noting water is incompressible, State 7 is the defined as:

$$h_{7s} = h_6 + v_6(p_7 - p_6) = 151.5 + 0.001(8000 - 6) = 159.5 \text{ kJ/kg}$$

$$h_7 = h_6 + \frac{h_{7s} - h_6}{\eta_p} = 151.5 + \frac{159.5 - 151.5}{0.7} = 162.9 \text{ kJ/kg}$$

State 8 is fixed by  $T_8 = 723$  K and  $p_8 = 8$  MPa:

$$h_8 = 3273 \text{ kJ/kg}$$
,  $s_8 = 6.557 \text{ kJ/kg} \cdot \text{K}$ 

Hence:

$$\alpha = \frac{h_4 - h_5}{h_8 - h_7} = \frac{1018 - 424.6}{3273 - 162.9} = 0.19$$

### b) Determine the work output of the gas and steam cycles: [12 points Undergrad | 18 points Grad]

For the gas cycle:

$$W_{net,GC} = W_{GT} - W_c$$
  
 $W_{GT} = h_3 - h_4$   
 $h_3 = 1636 \text{ kJ/kg}$ 

$$W_{GT} = h_3 - h_4 = 1636 - 1018 = 618 \text{ kJ/kg}$$

Similarly:

where:

$$W_c = h_2 - h_1$$

$$T_{2} = T_{1} \left( 1 + \frac{1}{\eta_{c}} \left[ \left( r_{p} \right)^{\frac{k-1}{k}} - 1 \right] \right) = 300 \left( 1 + \frac{1}{0.8} \left[ (8)^{\frac{0.39}{1.39}} - 1 \right] \right) = 597.1 \text{ K}$$
$$h_{1} = 300.4 \text{ kJ/kg}, h_{2} = 604.3 \text{ kJ/kg}$$

$$W_c = h_2 - h_1 = 604.3 - 300.4 = 303.9 \text{ kJ/kg}$$

Therefore:

$$W_{net,GC} = W_{GT} - W_c = 618 - 303.9 = 314.1 \text{ kJ/kg}$$

For the steam cycle (note  $p_9 = 6$  kPa and  $s_{9s} = s_8$ ):

$$h_{9s} = 2019 \, \text{kJ/kg}$$

$$h_{9} = h_{8} - \eta_{ST}(h_{8} - h_{9s}) = 3273 - 0.9(3273 - 2019) = 2144.4 \text{ kJ/kg}$$
$$W_{ST} = \alpha(h_{8} - h_{9}) = 0.19(3273 - 2144.4) = 214.4 \text{ kJ/kg}$$
$$W_{p} = \alpha(h_{7} - h_{6}) = 0.19(162.9 - 151.5) = 2.166 \text{ kJ/kg}$$
$$W_{net,SC} = W_{ST} - W_{p} = 214.4 - 2.166 = 212.2 \text{ kJ/kg}$$

The net work output of the combined cycle is:

$$W_{net} = W_{net,GC} + W_{net,SC} = 526.3 \text{ kJ/kg}$$

c) Determine the thermal efficiency of gas and steam cycles if they would operate separately: [4 points Undergrad | 6 points Grad]

The thermal efficiency of the gas turbine cycle alone is given by:

$$\eta_{th,GC} = \frac{W_{net,GC}}{q_{in}} = \frac{W_{net,GC}}{h_3 - h_2} = \frac{314.1}{1636 - 604.3} = 30.4\%$$

The thermal efficiency of the steam cycle alone is given by:

$$\eta_{th,SC} = \frac{W_{net,SC}}{\alpha(h_8 - h_7)} = \frac{212.2}{0.19(3273 - 162.9)} = 35.9\%$$

d) Determine the thermal efficiency of the combined cycle: [4 points Undrgrad | 6 points Grad]

The thermal efficiency of the combined cycle is:

$$\eta_{th,CC} = \frac{W_{net}}{q_{in}} = \frac{526.3}{1636 - 604.3} = 51\%$$

The efficiency of the combined cycle is much higher than that of the simple cycles.

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