

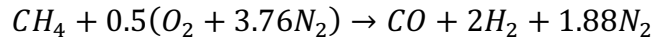
2.62 – Advanced Energy Conversion | Spring 2020

Homework 5 – Solutions

Problem 1 (40%)

A gas turbine power plant operates on pre-combustion CO₂ capture as shown in the figure provided. Determine the thermal efficiency of the cycle, and the outlet temperature of the turbine exhaust gas:

First, we start by noting the reaction occurring in the reformer: [15 points]



Applying the first law to the reformer:

$$Q_R = \sum_{\text{products}} H_i - \sum_{\text{reactants}} H_i$$

$$Q_R = \hat{h}_{CO}^{1073K} + 2\hat{h}_{H_2}^{1073K} + 1.88\hat{h}_{N_2}^{1073K} - (\hat{h}_{CH_4}^{298K} + 0.5\hat{h}_{O_2}^{298K} + 1.88\hat{h}_{N_2}^{298K})$$

The following thermodynamic properties have been used in the calculation:

Enthalpy of formations	Specific heat
$\hat{h}_{f,H_2O(g)}^o = -242 \text{ kJ/mol}$	$\hat{c}_{p,O_2} = 33.4 \text{ J/mol.K}$
$\hat{h}_{f,H_2O(l)}^o = -286 \text{ kJ/mol}$	$\hat{c}_{p,N_2} = 31.1 \text{ J/mol.K}$
$\hat{h}_{f,CO}^o = -110.6 \text{ kJ/mol}$	$\hat{c}_{p,CO_2} = 50.6 \text{ J/mol.K}$
$\hat{h}_{f,CO_2}^o = -393.8 \text{ kJ/mol}$	$\hat{c}_{p,H_2} = 30.0 \text{ J/mol.K}$
$\hat{h}_{f,CH_4}^o = -74.9 \text{ kJ/mol}$	$\hat{c}_{p,CO} = 29.3 \text{ J/mol.K}$
	$\hat{c}_{p,H_2O} = 38.2 \text{ J/mol.K}$
	$\hat{c}_{p,CH_4} = 46.35 \text{ J/mol.K}$

Taking the ambient conditions as the reference temperature, the heat supplied to the reformer is calculated to be:

$$Q_R = 78,820 \text{ kJ per kmol of } CH_4$$

For each kmol of methane fed to the reformer, 78820 kJ of heat should be supplied for the reforming of methane with air to occur.

Next, we analyze the air compressor using relationships from Chapter 5. The outlet temperature of the compressor is calculated as: [5 points]

$$T_{AC,o} = T_{AC,in} \left[1 + \frac{\left(\frac{p_o}{p_{in}}\right)^{\frac{k_{air}-1}{k_{air}}} - 1}{\eta_c} \right] = 298 \times \left[1 + \frac{10^{\frac{1.388-1}{1.388}} - 1}{0.75} \right] = 657 \text{ K}$$

Similarly, the first law is applied on one end of the heat exchanger yields: [15 points]

$$Q_{HEX} = (\hat{h}_{CO}^{1073K} - \hat{h}_{CO}^{673K}) + 2(\hat{h}_{H_2}^{1073K} - \hat{h}_{H_2}^{673K}) + 1.88(\hat{h}_{N_2}^{1073K} - \hat{h}_{N_2}^{673K})$$

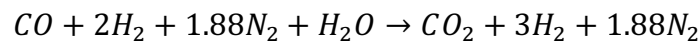
Note the reformat mixture should be leaving the HX at 673K (and not 573 K as mentioned in error by the problem statement).

$$Q_{HEX} = 59,107 \text{ kJ per kmol of CH}_4$$

Applying the first law on the other end of the heat exchanger yields Eq. 1:

$$Q_{HEX} = a(\hat{h}_{O_2}^{T_{HEX,o}} - \hat{h}_{O_2}^{T_{AC,o}}) + 3.76a(\hat{h}_{N_2}^{T_{HEX,o}} - \hat{h}_{N_2}^{T_{AC,o}})$$

In analyzing the shift reactor, we note the reaction occurring: [15 points]



By the first law:

$$Q_s = \hat{h}_{CO_2}^{308K} + 3\hat{h}_{H_2}^{308K} + 1.88\hat{h}_{N_2}^{308K} - (\hat{h}_{CO}^{673K} + 2\hat{h}_{H_2}^{673K} + 1.88\hat{h}_{N_2}^{673K} + \hat{h}_{H_2O}^{573K})$$

$$Q_s = -105,127 \text{ kJ per kmol of CH}_4$$

The heat requirement of the shift reactor is -105,127 kJ for each kmol of methane.

To analyze the separator compressor, we first need to determine the specific heat of the gas mixture: **[10 points]**

$$\hat{c}_{p, mix} = \sum_i \frac{n_i}{n_t} \hat{c}_{p,i} = \sum_i X_i \hat{c}_{p,i} = \frac{1}{5.88} \hat{c}_{p, CO_2} + \frac{3}{5.88} \hat{c}_{p, H_2} + \frac{1.88}{5.88} \hat{c}_{p, N_2} = 33.86 \text{ J/mol} \cdot \text{K}$$

$$k_{mix} = \frac{\hat{c}_{p, mix}}{\hat{c}_{p, mix} - 8.314} = 1.33$$

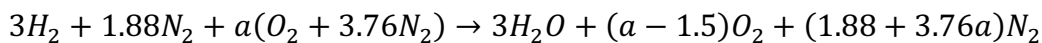
$$T_{Comp,o} = T_{Comp,in} \left[1 + \frac{\left(\frac{p_o}{p_{in}}\right)^{\frac{k_{mix}-1}{k_{mix}}} - 1}{\eta_c} \right] = 308 \times \left[1 + \frac{10^{\frac{1.33-1}{1.33}} - 1}{0.75} \right] = 624.5 \text{ K}$$

The work required by the process is calculated:

$$W_{SC} = (\hat{h}_{CO_2}^{624.5K} - \hat{h}_{CO_2}^{308K}) + 3(\hat{h}_{H_2}^{624.5K} - \hat{h}_{H_2}^{308K}) + 1.88(\hat{h}_{N_2}^{624.5K} - \hat{h}_{N_2}^{308K})$$

$$W_{SC} = 63,005 \text{ kJ per kmol of CH}_4$$

The next step is to analyze the combustor. We start by noting the reaction occurring: **[15 points]**



By the first law, we arrive at Eq. 2:

$$\begin{aligned} 3\hat{h}_{H_2}^{624.5K} + 1.88\hat{h}_{N_2}^{624.5K} + a(\hat{h}_{O_2}^{T_{HEX,o}} + 3.76\hat{h}_{N_2}^{T_{HEX,o}}) \\ = 3\hat{h}_{H_2O}^{1473K} + (a - 1.5)\hat{h}_{O_2}^{1473K} + (1.88 + 3.76a)\hat{h}_{N_2}^{1473K} \end{aligned}$$

Combining Equations 1 and 2 to solve for the unknowns a and $T_{HEX,o}$:

$$a = 5.238$$

$$T_{HEX,o} = 732.1 \text{ K}$$

Analyzing the gas turbine: [5 points]

$$\hat{c}_{p,mix} = \sum_i \frac{n_i}{n_t} \hat{c}_{p,i} = \sum_i X_i \hat{c}_{p,i} = \frac{3}{28.57} \hat{c}_{p,H_2O} + \frac{3.738}{28.31} \hat{c}_{p,O_2} + \frac{21.57}{28.31} \hat{c}_{p,N_2} = 32.11 \text{ J/mol} \cdot \text{K}$$

$$k_{mix} = \frac{\hat{c}_{p,mix}}{\hat{c}_{p,mix} - 8.314} = 1.35$$

$$T_{T,out} = T_{T,in} \left(1 - \eta_T \left[1 - (r_p)^{\frac{1-k_{mix}}{k_{mix}}} \right] \right) = 1473 \left(1 - 0.88 \left[1 - (0.1)^{\frac{1.35-1}{1.35}} \right] \right) = 890.3 \text{ K}$$

$$W_T = 3(\hat{h}_{H_2O}^{1473K} - \hat{h}_{H_2O}^{890.3K}) + 3.738(\hat{h}_{O_2}^{1473K} - \hat{h}_{O_2}^{890.3K}) + 21.57(\hat{h}_{N_2}^{1473K} - \hat{h}_{N_2}^{890.3K})$$

$$W_T = 530,521 \text{ kJ per kmol of CH}_4$$

The net work produced by the power cycle may be calculated according to: [2.5 points]

$$W_{net} = W_T - W_{AC} - W_{SC}$$

where

$$W_{AC} = 5.238(\hat{h}_{O_2}^{657K} - \hat{h}_{O_2}^{298K}) + 19.69(\hat{h}_{N_2}^{657K} - \hat{h}_{N_2}^{298K}) = 282,707 \text{ kJ per kmol of CH}_4$$

Therefore:

$$W_{net} = 530,521 - 282,707 - 63,005 = 184,809 \text{ kJ per kmol of CH}_4$$

For every kmol of methane used in the system, 184,809 kJ net power is produced.

The thermal efficiency of the power cycle is therefore obtained as: [2.5 points]

$$\eta_{th} = \frac{W_{net}}{M_{CH_4} LHV} = \frac{184,809}{16 \times 50050} = 23.1\%$$

To determine the turbine exhaust temperature, we write the following equation: **[15 points]**

$$3 \left(\hat{h}_{H_2O}^{890.3 K} - \hat{h}_{H_2O}^{T_{g,out}} \right) + 3.738 \left(\hat{h}_{O_2}^{890.3 K} - \hat{h}_{O_2}^{T_{g,out}} \right) + 21.57 \left(\hat{h}_{N_2}^{890.3 K} - \hat{h}_{N_2}^{T_{g,out}} \right) = Q_R + Q_S + Q_B$$

where:

$$\begin{aligned} Q_B &= \left(\hat{h}_{H_2O}^{573 K} - \hat{h}_{H_2O}^{298 K} \right) = (\Delta H_v + \Delta H_s) \\ &= (40,650 \text{ kJ} + 75.3\{373 - 298\} + 38.2 \{573 - 273\}) \\ &= 57,757.5 \text{ kJ per kmol of CH}_4 \end{aligned}$$

Therefore:

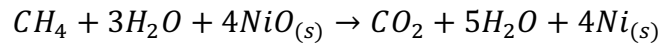
$$T_{gas,out} = 856.4 \text{ K}$$

The thermal efficiency is rather low; this is a simple cycle. The poor efficiency is because of the low pressure ratio and lower maximum, temperature in the gas turbine cycle, CO2 separation and the several heat transfer irreversibility in the heat transfer components. Adding a steam cycle as a bottoming cycle could raise the efficiency.

Problem 2 (60%)

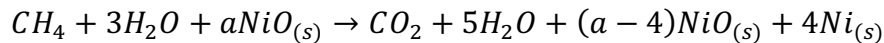
- a) Determine the composition of the chemical loop and the fuel exhaust stream at the exit of the reduction reactor: [25 points]

We start by noting the chemical reaction within the reduction reactor is:



Note that the fuel exhaust stream is $CO_2 + 5H_2O$.

Denoting a as the number of moles entering the oxidation reactor:



Using the definition of the degree of reaction:

$$X_{red} = \frac{m - m_{Red}}{m_{Ox} - m_{Red}} = \frac{[(a - 4)M_{NiO} + 4M_{Ni}] - aM_{Ni}}{aM_{NiO} - aM_{Ni}} = 0.3$$

Noting that $M_{NiO} = 74.7$ kg/kmol and $M_{Ni} = 58.7$ kg/kmol, and solving for a , we arrive at:

$$a = 5.714$$

In other words, 70% of the NiO entering the reduction reactor is reacted with one mole of methane. So, 5.714 moles of NiO enters the reduction reactor and 1.714 moles of NiO leaves unreacted.

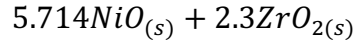
Noting that the mass ratio of NiO to YSZ is 3:2 when $X = 1$:

$$\frac{(nM)_{NiO}}{(nM)_{YSZ}} = \frac{3}{2} \Rightarrow \frac{n_{YSZ}}{n_{NiO}} = \frac{2}{3} \left(\frac{M_{NiO}}{M_{YSZ}} \right) = \frac{2}{3} \times \frac{74.7}{123.2} = 0.4$$

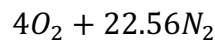
Hence, the number of moles of ZrO_2 is $n_{YSZ} = 0.4 \times 5.714 = 2.3$, and the chemical loop composition is $1.714NiO_{(s)} + 4Ni_{(s)} + 2.3ZrO_{2(s)}$.

- b) Determine the composition of the chemical loop and the air stream at the exit of the oxidation reactor: [10 points]

The composition of the chemical loop into the reduction reactor only includes NiO since $X_{Ox} = 1$. All Ni is oxidized to NiO in the oxidation reactor, and the composition is given by:



For the air stream: $4Ni_{(s)} + 2O_2 \rightarrow 4NiO_{(s)}$. Thus, 2 moles of O_2 (out of the 6 supplied) are used to oxidize Ni(s). The composition of the exit air stream is:



- c) Determine the temperature of air at the inlet of the oxidation reactor: [15 points]

Applying the first law to the oxidation reactor:

$$\begin{aligned} (6h_{O_2}^T + 22.56h_{N_2}^T) + (1.71h_{NiO}^{900K} + 4h_{Ni}^{900K} + 2.3h_{ZrO_2}^{900K}) \\ = (4h_{O_2}^{1500K} + 22.56h_{N_2}^{1500K}) + (5.71h_{NiO}^{1500K} + 2.3h_{ZrO_2}^{1500K}) \end{aligned}$$

$$\begin{aligned} 4\Delta h_{Ox}^{1500K} = (6c_{p,O_2} + 22.56c_{p,N_2})(1500 - T) \\ + (1.71c_{p,NiO} + 4c_{p,Ni} + 2.3c_{p,ZrO_2})(1500 - 900) \end{aligned}$$

The exothermic enthalpy of the reaction is used to heat up the reactants to the oxidation reactor temperature, 1500K. A solution of the above yields:

$$T = 759.5 \text{ K}$$

- d) Determine the temperature of the chemical loop at the inlet of the reduction reactor: [15 points]

Applying the first law to the reduction reactor:

$$\begin{aligned} (h_{CH_4}^{730K} + 3h_{H_2O}^{730K}) + (5.71h_{NiO}^T + 2.3h_{ZrO_2}^T) \\ = (1.71h_{NiO}^{900K} + 4h_{Ni}^{900K} + 2.3h_{ZrO_2}^{900K}) + (h_{CO_2}^{900K} + 5h_{H_2O}^{900K}) \end{aligned}$$

$$\Rightarrow \Delta h_{Red}^{900K} + (c_{p,CH_4} + 3c_{p,H_2O})(900 - 730) = (5.71c_{p,NiO} + 2.3c_{p,ZrO_2})(T - 900)$$

The inlet stream is cooled down to 900 K by the endothermic reduction reaction and by heating up the fuel stream to 900 K. Solving the above equation, we arrive at:

$$T = 1246 \text{ K}$$

e) Determine the temperature at the exit of heat exchanger 2: [10 points]

Applying the first law to heat exchanger 2 yields:

$$(c_{p,CO_2} + 5c_{p,H_2O})(T - 900) = (5.71c_{p,NiO} + 2.3c_{p,ZrO_2})(1500 - 1246)$$

Solving for the exit temperature we arrive at:

$$T = 1392 \text{ K}$$

f) Determine the thermal efficiency of the plant with 100% CO₂ recovery rate, assuming a liquefaction work of 20 kJ per mole of methane: [25 points]

The thermal efficiency of the plant is calculated as:

$$\eta_{th} = \frac{W_{T_1} + W_{T_2} - W_c - W_{liq}}{LHV_{CH_4}}$$

In this calculation, we note (specific heats calculated as in Problem 1):

$$W_{T_1} = n_1 \eta_T c_{p,1} T_{in} \left(1 - \pi_p^{-R/c_p}\right) = 26.56 \times 0.9 \times 32.43 \times 1500 \times \left(1 - 20^{-\frac{8.314}{32.43}}\right) = 623,341 \text{ J}$$

$$W_{T_2} = n_2 \eta_T c_{p,2} T_{in} \left(1 - \pi_p^{-R/c_p}\right) = 6 \times 0.9 \times 42.15 \times 1392 \times \left(1 - 20^{-\frac{8.314}{42.15}}\right) = 141,362 \text{ J}$$

$$W_c = \frac{n_3 c_{p,3} T_{in}}{\eta_c} \left(\pi_p^{R/c_p} - 1\right) = \frac{28.56 \times 32.56 \times 298}{0.8} \left(20^{8.314/32.56} - 1\right) = 397,960 \text{ J}$$

Consequently:

$$\eta_{th} = \frac{623,341 + 141,362 - 397,960 - 20,000}{16 \times 50,050} = 43\%$$

MIT OpenCourseWare
<https://ocw.mit.edu/>

2.60J Fundamentals of Advanced Energy Conversion
Spring 2020

For information about citing these materials or our Terms of Use, visit: <https://ocw.mit.edu/terms>.