1. Operating Parameters

Summary

Position	Temp (K)	Pressure (bar)	Composition
1	288.15	1.013	91.3% Methane, 5.36% Ethane, 2.83% Nitrogen, 0.5% CO2 and 0.01% O2
2	288.15	1.013	78.08% N2, 20.95% O2 and 0.93% Ar
3	692	23.299	78.08% N2, 20.95% O2 and 0.93% Ar
4	536	23.299	91.3% Methane, 5.36% Ethane, 2.83% Nitrogen, 0.5% CO2 and 0.01% O2
5	536	23.299	91.3% Methane, 5.36% Ethane, 2.83% Nitrogen, 0.5% CO2 and 0.01% O2
6	838.65	23.88654	100% H2O(g)
7	1073.1	23.299	45% H2, 36% H2O(g), 7% CO, 6% CO2, 5% CH4, 0.5% N2, Neg. NOx
8	1173.1	23.299	51% N2, 28% H2O(g), 7% O2, 5% H2, 3% CO, 3% CO2, 2% CH4, Neg. NOx
9	692	23.299	78.08% N2, 20.95% O2 and 0.93% Ar
10	1073.15	23.299	78.08% N2, 20.95% O2 and 0.93% Ar
11	1940.9	23.299	78.08% N2, 20.95% O2 and 0.93% Ar
12	1737	23.299	61% N2, 29% H2O(g), 7% CO2, 3% O2 , 0.2% NO, Neg. other NOx
13	692	23.299	61% N2, 29% H2O(g), 7% CO2, 3% O2 , 0.002% NO, Neg. other NOx
14	1852.9	21.43508	61% N2, 29% H2O(g), 7% CO2, 3% O2 , Neg. NOx
15	1011.528959	1.039338	100% H2O(g)
16	428.15	1.02313	100% H2O(g)
17	838.65	123.586	100% H2O(g)
18	586.7338269	23.88654	100% H2O(g)
19	838.65	23.88654	100% H2O(g)
20	838.65	23.88654	100% H2O(g)
21	513.4686376	2.36029	100% H2O(g)
22	292.15	2.0062465	100% H2O(l)
23	283.15	1.013	100% H2O(l)
24	321.15	130.0905263	100% H2O(l)
25	536	23.299	91.3% Methane, 5.36% Ethane, 2.83% Nitrogen, 0.5% CO2 and 0.01% O2

Analysis

The following parameter information was given by the coursework sheet:

Position	Temp (K)	Pressure (bar)
1	288.15	1.013
2	288.15	1.013
15	0	1.039338
16	428.15	1.02313
17	838.65	123.586
18	0	23.88654
19	838.65	0
21	0	2.36029
22	292.15	0
23	283.15	1.013
24	321.15	0

Position	Mass (kg/s)
1	23.9
2	598.7
5	17.9
13	254.7

Mass was calculated from the last 2 digits of CID following the prescribed formula.

Flow 25 was defined as the flow from the NG compressor straight to the combustor.

Steam cycle

Assuming all pipes have no pressure loss and all interconnected pipes share intensive properties and composition.

Pumps: Starting at 22 we determine the pressure of the state from calculating the outlet pressure of the condenser given a pressure loss of 15% (*given by coursework*) and the pressure before condenser at 21. $P_{22} = 0.85 * P_{21} = 0.85 * 2.33atm = 2.36 \, bar$. Then given that pump 2 is isentropic (*given by coursework*) using isentropic relations the temperature at 23 was determined from state 23 with:

$$\Delta s = C_p \ln\left(\frac{T_2}{T_1}\right) - R \ln\left(\frac{P_2}{P_1}\right) \quad \&\& \quad \Delta s = 0 \rightarrow T_2 = T_1 \left(\frac{P_2}{P_1}\right)^{\frac{R}{C_p}}$$

Pressure at 24 was calculated by inverting the pressure loss of 5% across the HRSG along flow 24-17. $P_{24} = \frac{P_{17}}{0.95} = 130 bar$.

Turbines: Given state 17, state 18 was determined through the polytropic efficiency (*89% given by coursework*). This was converted to isentropic efficiency using a reheat factor of 1.07 (relationship derivation and validity of value chosen for steam turbine given by (Dixon, 2010)) $\eta_{isen} = \eta_{poly} * r_{reheat}$.

Using the isentropic efficiency/enthalpy definition for turbines $\eta_{isen} = \frac{\Delta h}{\Delta h_{isen}}$, the enthalpy of the product was determined. Using the enthalpy determined, coupled with the pressure at 18 (*given by coursework*) the temperature at 18 was found using a steam table.

The pressure at position 19 was determined by carrying through the pressure at 18 (*assuming no pressure loss as it is superheated vapour and the gas side experienced nearly no pressure loss across a much larger temperature range*).

Using the completed state of 19, state 20 and state 6 were determined to have the same properties (*assuming connected pipes share intensive properties*).

Using state 20, the isentropic efficiency was determined using the reheat factor (again taken as 1.07) and polytropic efficiency (*given as 89%*) and used again to determine output enthalpy and thus determine output temperature, given the pressure of 21 being supplied by the coursework.

Natural Gas cycle

Compressor: As natural gas is not a perfect gas (C_p varies throughout the approximate temperature range, tested through GASEQ) GASEQ was used to adiabatically compress the natural gas (*which was taken as 91.3% Methane, 5.36% Ethane, 2.83% Nitrogen, 0.5% CO_2 and 0.01% O_2 – this was determined through filling the miscellaneous components by looking at major constituents from* (Union Gas, 2018)) to $23atm$ and thus determine state 4. There was insignificant specific entropy change and as such GASEQ was used to model the isentropic compression (*given by the coursework*).

Reformer: Given state 4, state 5 and 6 were taken to have the same intensive properties and composition due to being connected. Given state 6 (*calculated as above*) the composition of flow 5 and 6 was put into GASEQ, following a specified molar ratio of steam: carbon (*given as 3 by coursework*) at an isothermal temperature (800°C) and equilibrium was calculated for state 7. The pressure of 5 was used as the pressure of 6 was within 2% of the value and as such the resultant pressure would stay approximately the same.

Fuel Cell: Given state 10 (*calculated as below*) the reaction at the fuel cell enabled deduction of state 8. Using the overall chemical equilibrium equation below, the composition of the flows was changed.

$$H_2 + \frac{1}{2}O_2 \leftrightarrow H_2O + 2e^-$$
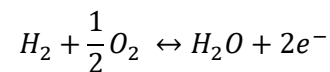
This was achieved by determining an incoming molar flowrate of hydrogen reacting (*mass fraction given by GASEQ, overall mass flowrate of 7 calculated as below and molar weight of hydrogen used to convert*) and multiplying it by the fuel utilisation (*given by coursework*). Given the molar flowrate of hydrogen reacting a molar flowrate of oxygen and water used/produced in the reaction by multiplying by relative moles from above eqn. This was then subtracted (for H_2 and O_2) or added (for H_2O) from the molar flowrate of each respective constituent (obtained as the hydrogen mole flowrate was above but in stream 10 for O_2 and stream 7 for H_2O and H_2) coming in. As all composition analysis was done fractionally in GASEQ, molar flowrate fractions were used to make sure all ratios put in the new set of products had the correct ratios. E.g. $O_{2,stream\ 8}/H_{2,stream\ 8}$ was used to determine the relative moles of O_2 as a multiple of the H_2 in the output stream. The fuel cell was assumed to be constant pressure and constant temperature to determine state 8.

Afterburner: It was assumed that there was insufficient time between leaving the fuel cell and entering the combustor for the products to reach equilibrium – thus the molar ratios calculated as above were taken as the incoming composition. GASEQ was used to analyse the composition at 8 as the reactant side of an adiabatic equilibrium at constant pressure (*assuming sufficiently slow burning that it can be modelled as a const. pressure combustion*) at the input state given by position 8. This determined the output temperature and fixed state 11 as well as the composition.

Heat Exchanger: The specific enthalpy of position 11 was determined from GASEQ given pressure and temp. and the enthalpy at state 12 was determined by using the insulated nature of the heat exchanger (*given by coursework*) and thus balancing the rise in actual enthalpy of flow 9 to 10 (*as calculated below*) against flow 11 to 12 (*assuming no work in the heat exchanger*). Given a specific enthalpy (*dividing actual enthalpy by mass flowrate of 11 as determined below*) and pressure at state 12 (*assuming no pressure loss across the heat*

exchanger), GASEQ was used to manually iterate state 12 temperature given the composition to achieve the specific enthalpy decrease required.

Air cycle

Compressor: Given state 2 (*by coursework*) – state 3 was determined using GASEQ, with an adiabatic compression for a pressure ratio (*given by coursework*) and checking the change in specific entropy is negligible to confirm the isentropic resultant nature. Although technically a perfect gas it was decided that using GASEQ would be more accurate as ultimately there is no real perfect gas and as such it is was assumed it is better to avoid perfect gas relations unless necessary. The composition of air was assumed to be 78.08% N_2, 20.95% O_2 and 0.93% Ar (University Corporation of Atmospheric research, 2018).

Given state 3 the intensive properties of state 9 and 13 were assumed to be the same as the share a pipe connection.

Combustor: The molar composition of flow 13, 25 and 12 was saved into a mixture in GASEQ and then using mass flowrates for each (*as calculated per below*) molar flowrates were determined through division of $\dot{m}_n$ by mean molecular weight, M_n of each flow mixture and used to determine the ratio of moles of each flow in GASEQ. The flows were then set to their respective temperatures in GASEQ and an adiabatic process at constant pressure was performed to determine the chemical composition and state of 14. This assumes the combustion is slow enough that the process occurs at constant pressure and that the pressure loss due to the combustor happens after the combustion, perhaps due to increased turbulence from combustion and head loss as it travels through pipes.

Turbine: State 15 was determined by using the polytropic efficiency (*given by coursework*) and the perfect gas polytropic efficiency relationship (*given by Appendix of ME3 TDE notes*). Given the pressure at 15 (*given by coursework*) and the pressure, temperature and gamma of 14 (*given by composition of 14 from GASEQ, and assuming const. gamma*), the formula was rearranged and used:

$$\eta_{polytropic} = \frac{\gamma - 1}{\gamma} * \frac{\ln\left(\frac{P_2}{P_1}\right)}{\ln\left(\frac{T_2}{T_1}\right)} \rightarrow T_2 = T_1 e^{\frac{\gamma-1}{\gamma}\ln\left(\frac{P_2}{P_1}\right)}$$

It is worth noting that this is likely the least accurate assumption of the whole analysis due to the C_p of the combustor products varying largely with temp and pressure differences (drops in order of ~15%) and as such cannot really be considered a perfect gas. However, as reheat relationships for gas turbines could not be found in the literature, the formula was used.

Mass flowrates

Mass flowrates were determined through conservation of mass and given mass flowrate at state 1,2,5 and 13 (*by coursework*) for the air and steam cycle. This can be summarised in:

NG compressor flows $\dot{m}_1 = \dot{m}_4 = \dot{m}_5 + \dot{m}_{25}$

SOFC and Reformer $\dot{m}_{10} = \dot{m}_9 = \dot{m}_3 - \dot{m}_{13}; \dot{m}_7 = \dot{m}_5 + \dot{m}_6; \dot{m}_8 = \dot{m}_{10} + \dot{m}_7 = \dot{m}_{11} = \dot{m}_{12}$

Combustor cycle $\dot{m}_3 = \dot{m}_2; \dot{m}_{14} = \dot{m}_{12} + \dot{m}_{13} + \dot{m}_{25} = \dot{m}_{15} = \dot{m}_{16}$

$\dot{m}_6$ (and $\dot{m}_{23}$ which is used to make up for the loss from the steam cycle) is determined through converting molar flowrate needed for the steam:carbon ratio (*given by coursework*)as given above into a mass through molecular weight:

$$\dot{m}_6 = \dot{N_{needed}} M_{H2O} = \dot{N_{H_2}} * r_{steam:carbon} M_{H2O} \ (= \dot{m}_{23})$$

The remaining mass flowrate throughout the steam cycle can be determined through SFEE on the HRSG, using drops in enthalpy from GASEQ and the steam tables, and assuming mass flowrate through 18 to 19 and 17 to 18 is the same:

$$\dot{m}_{24,17,18,19} = \frac{\dot{m}_{15}\Delta h_{16,15}}{\Delta h_{19,18} + \Delta h_{17,18}} \rightarrow \dot{m}_{22,21,20} = \dot{m}_{19} - \dot{m}_6$$

2. Fuel Cell Performance

Summary

Volts per cell	$0.37V$
AC power of SOFC	$117.5MW$
Fuel cell efficiency at nom. conditions	$\eta_{voltage} = 21\%$
Active area of fuel cell	$68282m^2$
Net Heat loss in SOFC	$37.4MW$

Volts per Cell

Using the Nernst potential equation (*given by TDE notes*):

$$E = E_0 - \frac{RT}{zF} \ln\left(\frac{\prod X_{product}^A}{\prod X_{reactant}^A}\right) - \frac{RT}{zF} \ln\left(\frac{P}{P_0}\right)$$

$$z = electrons\ released\ per\ mol\ of\ reaction; F = Faraday\ const.; P_0 = Atmospheric\ pressure;$$

$$X = mole\ ratio\ for\ whole\ mixture; \ A = relative\ moles\ per\ mole\ of\ the\ reaction$$

$$E_0 = -\frac{\Delta \overline{g_0}}{zF} = -\frac{\Delta \overline{h_{0,reaction}} - T\Delta \overline{s_{0,reaction}}}{zF} = \frac{\sum_{products}(\Delta \overline{h_0} - T\Delta \overline{s_0}) - \sum_{reactants}(\Delta \overline{h_0} - T\Delta \overline{s_0})}{zF}$$

$$\overline{\Delta h_0} = standard\ molar\ enthalpy\ of\ formation; \ \overline{\Delta s_0} = standard\ molar\ entropy$$

Given the chemical composition of inlets and outlets and states (*as calculated per above*) the ideal Nernst voltage was calculated. Then using Figure 1 the ohmic and activation losses were determined at the nominal temp (*given as 900°C by coursework*). The losses were then subtracted from the ideal Nernst voltage.

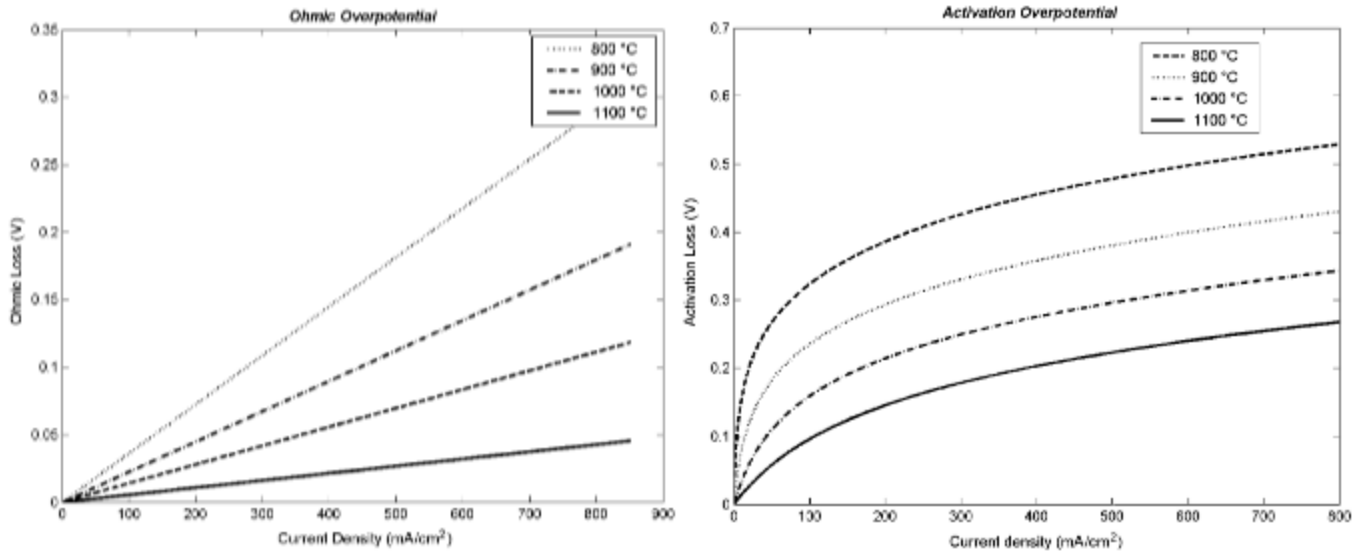$$V_{real} = E - V_{ohmic} - V_{activation}$$

Figure 1 Ohmic and Activation losses in SOFC as function of temperature

AC power

The AC power was determined from:

$$P_{AC} = \eta_{AC/DC}P_{DC} = \eta_{AC/DC}IV_{real} = \eta_{AC/DC}\dot{C}_{reacts}V_{real} = \eta_{AC/DC}\frac{\dot{N}_{H2\,react}}{zF}V_{real}$$

Where $\dot{N}_{H2\,reacts}$ was the molar flowrate of hydrogen reacting in the fuel cell as obtained from the SOFC analysis as above.

Fuel cell efficiency

Fuel cell efficiency was evaluated through voltage efficiency (*given by TDE notes*) with it being a more useful indicator of the useful efficiency coming out as usable voltage and current.

$$\eta_{Volt} = r_{fuel\,util}\frac{V_{real}}{E_{max}} \; where \; E_{max} = \frac{\Delta\overline{h_0}}{zF}$$

Active area

The active area of the fuel cell was determined through the current calculated and the current density given by the coursework:

$$A = \frac{I}{\rho_{current}} = 68\,828$$

Heat losses

Net heat loss of the SOFC was obtained through a rearranged SFEE on the reformer and fuel cell, as other components where assumed adiabatic (*given by coursework*):

$$\Delta\dot{Q}_{net} = \Delta\dot{Q}_{reformer} + \Delta\dot{Q}_{cell\,reaction} + \Delta\dot{Q}_{cell\,losses} = -37.4MW$$

Where, ignoring activation losses as they are not given to the surrounding but rather to the reaction:

$$\Delta \dot{Q}_{reformer} = \Delta \dot{H} = \dot{m}_7 h_7 - \dot{m}_6 h_6 - \dot{m}_5 h_5 = 0.2MW$$

$$\Delta \dot{Q}_{cell\ reaction} = \left(\Delta \dot{H} - \Delta \dot{G}\right)_{reaction} = T\Delta \dot{S}_{reaction} = T\left[\sum \dot{N}_i \Delta \bar{s}_i\right]_{out-in} = -0.09MW$$

$$\Delta \dot{Q}_{cell\ losses} = IV_{ohmic} = -37.6MW$$

3. System Parameters

Power

The net power of the system was obtained through the sum of enthalpy changes across compressors, pumps, turbines -assuming all to be enthalpy drop to correspond to work gains (a.k.a. adiabatic) and the AC power of the fuel cell system. Also accounting for the units of enthalpy being $\frac{kJ}{kg}$. This gave a net power of $763.2MW$.

$$\dot{W}_{net} = \dot{W}_{AC} - \sum_i \dot{m}_i(h_i - h_j = 763.2MW$$

$$where\ i \in \{4,3,15,18,21,22,24\}\ and\ h_j\ refers\ to\ flow\ physically\ before\ the\ i^{th}$$

Feed-water

Feed water was assumed to mean the water required to be supplied to the system during runtime to maintain functionality. This can be seen by inspection to be the water leaving the steam cycle in flow 6, and as such:

$$\dot{m}_{feed\ water} = \dot{m}_6 = 55.9kgs^{-1}$$

Efficiency

For such a complex system, the most meaningful efficiency can be derived by going by to the root concept of efficiency. Assuming the only source of energy for the system is given by the supply of fuel as all other heat intake is internal to the system as whole, and the feed water is never brought below the supply temperature meaning heat is not extracted from surrounding water. Furthermore, from a design perspective our primary source of energy contribution can be viewed as just the fuel as it is all we supply that costs significantly. This efficiency came out to be:

$$\eta_{system} = \frac{Work\ out}{Energy\ in} = \frac{\dot{W}_{net}}{\dot{H}_{fuel}} = \frac{\dot{W}_{net}}{\dot{m}_1 LHV} = 68.1\%$$

Emissions

CO$_2$

Emissions were determined from:

$$\epsilon_{CO2} = \frac{\dot{m}_{16} r_{CO2}^{mass}}{W_{out}} = 360 \frac{g}{kWh}$$

Where r_{CO2}^{mass} is the mass fraction of CO_2 in the emission at position 16 (from GASEQ) and W_{out} is in units of kWh.

NO$_x$

And using the same method but with the cumulative mass fraction of NO_x:

$$\epsilon_{CO2} = \frac{\dot{m}_{16} r_{NOx}^{mass}}{W_{out}} = 2.45 \; \frac{\mu g}{kWh}$$

It is worth noting that this is exceptionally low and was calculated assuming there was enough time to reach equilibrium in between each stage after the combustion (including the pressure loss). It is worth noting that the emissions that come straight out of the turbine would cause ~2 $\frac{g}{kWh}$ which when compared with the literature (J. A. de Gouw, 2014) is approximately the same order of magnitude as a CCP Natural gas power plant.

Appendix

Table 1 Mass flowrates of all positions

	Mass (kg/s)			
1	23.9		15	678.56989
2	598.7		16	678.56989
3	598.7		17	132.4402616
4	23.9		18	132.4402616
5	17.9		19	132.4402616
6	55.96988998		20	76.47037159
7	73.86988998		21	76.47037159
8	417.86989		22	76.47037159
9	344		23	55.96988998
10	344		24	132.4402616
11	417.86989		25	6
12	417.86989			
13	254.7			
14	678.56989			

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