



Norwegian University  
of Life Sciences

Master's Thesis 2016

30 ECTS

Department of Mathematical Sciences and Technology

# **A Model for the Zero Emission Gas Technology as a Tool for Process Optimization**

**Daud Malik**

Environmental Physics and Renewable Energy

## Acknowledgements

I want to thank everybody who helped me during this exciting process.

First of all, I want to thank Dr. Nicola Di Giulio, my supervisor at ZEG Power®, for dedicated and excellent guidance throughout the semester. Nicola contributed with good advice and was always there to point me in the right direction. His knowledge in physics, ZEG-technology and simulation techniques was invaluable. This semester would not be complete without his help, he is truly an “a buon rendere” as they say in Italy. Further, I want to thank Dr. Espen Olsen, my supervisor at NMBU, for valuable advice.

I also want to thank Dr. Bjørg Andresen, at ZEG Power® for her editorial advice, memorable chats and for giving me the opportunity to write the thesis. Also, the guys from HYSTORSYS AS, Jon Eriksen and Roman Densys, are to be thanked for making my stay at Villa Sole memorable.

I want to thank Jorge Marchetti at NMBU for his guidance regarding chemical engineering.

I am also thankful for having the chance to work in the same building as the great scientists that work at ZEG Power®, and for getting to learn more about the different research fields within hydrogen technology.

Thanks to my friends at IFE and NMBU, especially Ingvild Veddeng, for contributing with constructive discussion and good times throughout this semester. Team Eagle and DÅs will forever be a part of me.

At last, I want to thank my parents, Rubeena Malik and Hamayun Kabir Malik, the two most loving people in my world, and my family, for being supportive and loving.

NMBU, Ås, 14.12.2016

Daud Malik



## Abstract

The ZEG-technology (Zero Emission Gas - ZEG<sup>®</sup>) is highly efficient technology for co-production of hydrogen and electric power with integrated CO<sub>2</sub> capture.

The purpose of this study is to simulate the ZEG-technology in order to obtain a simplified model, which is used to understand the behaviour of ZEG plants in different configurations. This is important for initial evaluation of system design for different technology applications.

ZEG Power utilizes a combination of two core technologies, Sorption Enhanced Reforming (SER) and Solid Oxide Fuel Cells (SOFC). SER is a modified reforming technology for hydrogen production with integrated CO<sub>2</sub> capture. The SOFC is a technology that generates electrical power from hydrogen at a high efficiency (~60%).

A zero-dimensional model for preliminary studies of the ZEG-technology in different configurations is made using the Engineering Equation Software (EES software). For the simulation of the technology, energy balance is taken into account. The simulation is set to result in different dependent variables, and compared to previous simulations of the ZEG-technology. The comparison is executed in order to verify the quality of the model made in EES. In addition, sensitivity analysis is performed in order to show the capacity of the ZEG-technology upon varying some of the independent variables in the simulation.

When comparing the EES model with previous simulations, relative good results were achieved. The highest deviation from the most updated previous simulations was at 3,3%, which is not a significant value, considering that the previous simulations were more comprehensive. The sensitivity analysis showed the functioning of the EES model, and the tested dependent variables reacted accordingly upon changing the independent variables.



## Sammendrag

ZEG-teknologien (Zero Emission Gas Power, ZEG<sup>®</sup>) er en høyeffektiv hybrid teknologi som driver samtidig produksjon av hydrogen og elektrisitet med integrert CO<sub>2</sub> fangst.

Formålet med denne oppgaven er å lage en simuleringsmodell for ZEG-teknologien, som kan brukes til å forstå virkemåten til kraftsystemet i forskjellige konfigurasjoner. Dette er viktig når en skal foreta forstudier for ZEG-teknologien i forskjellige applikasjoner.

ZEG Power tar i bruk to teknologier, Sorption-Enhanced Reforming (SER) og Solid Oksid Brenselcelle (SOFC). SER er et reaktorsystem for hydrogenproduksjon med integrert CO<sub>2</sub> fangst. SOFC er en høytemperatur brenselcelle som generer elektrisk kraft fra hydrogen med en høy effektivitet (~60%).

En nulte dimensjons modell for ZEG-teknologien er lagd i programmet Engineering Equation Solver (EES). For selve simuleringen er energibalanse og kjemisk likevekt tatt i betraktning. Simulasjonen skal i hovedsak gi forskjellige resultater for de betraktede avhengige variablene som er i etterkant blir sammenlignet med tidligere simulasjoner på ZEG-teknologien. Sammenligningen er utført for å validere om modellen besitter god kvalitet for ZEG-teknologien. Det er også utført sensitivitets analyse for å undersøke kapasiteten til ZEG-teknologien. Dette er utrettet ved å variere de uavhengige variablene i modellen for så å se reaksjonen i de avhengige variablene.

Ved sammenligning av modellen mot de mest oppdaterte eldre simulasjonene, ble gode resultater oppnådd. Det høyeste avviket er observert til å være 3,3%. Dette avviket er ikke høyt når en tar hensyn til hvor omfattende de tidligere modellene er. Sensitivitets analysen viste at modellen fungere i forhold til det en forventer av ZEG-teknologien.



# Contents

Acknowledgements .....	i
Abstract .....	iii
Sammendrag .....	v
List of figures .....	viii
List of tables.....	ix
Abbreviations .....	x
Symbols .....	xi
1 Introduction.....	1
1.1 Background and motivation .....	1
2. The ZEG-technology.....	3
2.1 Introduction.....	3
2.2.1 Reformer.....	4
2.3 Solid Oxide Fuel Cell (SOFC).....	6
3. Simulation.....	11
3.1 Model theory.....	11
3.1.1 Equilibrium .....	11
3.1.2 First law of thermodynamics.....	12
3.2 Engineering equation solver (EES).....	13
3.2.1 Guess value, upper and lower limits .....	15
3.1.2 Built-in functions .....	15
3.3 Previous work.....	16
3.4 Simulation of the ZEG-technology.....	17
3.4.1 Sorption-Enhanced reforming.....	19
3.4.4 SOFC.....	22
4. Simulation performance.....	25
4.1 Model validation.....	27
4.1 Sensitivity analysis.....	29
5. Conclusion .....	37
6. Further work.....	39
References.....	41
Appendix A .....	43
Appendix B .....	47
Appendix C .....	61
Appendix D .....	65



## List of figures

Figure 1. Simplified scheme of the ZEG-technology [3].	3
Figure 2. Simplified scheme of the SER system [4].	4
Figure 3. Thermodynamic equilibrium for conventional SMR and SER [6].	5
Figure 4. General description of SOFC function [12].	7
Figure 5. Yttrium-Stabilized Zirconia molecule 3-D structure [13].	7
Figure 6. Stack configuration of a planar SOFC [12].	8
Figure 7. The operational losses through an electrolyte when increasing the current density [11].	9
Figure 8. Graphic illustration of equilibrium[18].	11
Figure 9. Example of a diagram created in EES [21].	14
Figure 10. Example of a parametric table and plot for the function $y = 2*x$	15
Figure 11. Example of calling the heat capacity of a substance in EES	16
Figure 12. Basic model design for the chose ZEG configuration	17
Figure 13. Box surface of the simulation model.	18
Figure 14. The control surface of the SER for the simulation in EES	19
Figure 15. Control surface for the SOFC.	22
Figure 16. A schematic of the model setup for the catalytic burner in EES	24
Figure 17. Program made in EES for illustration of model and interactive simulation of the ZEG Power technology. This diagram show the output of the simulation on the ZEG400 configuration.	26
Figure 18. Plot of composition of CO <sub>2</sub> in biogas versus the inlet temperature of the reformer	30
Figure 19. Plot of the heat loss in the regenerator against the heat need of the regenerator and the standalone efficiency of the SER.	31
Figure 20. Plot of the fuel utilization of the SOFC against the efficiency of co-generation	32
Figure 21. Plot of the co-generation efficiency with varying oxygen utilization	33
Figure 22. Plot of the efficiency of standalone generation versus the temperature at the inlet of the catalytic burner	34
Figure 23. Plot of the effect of oxygen utilization on the cathodic inlet temperature	35
Figure 24. The influence of the SOFC temperature on the co-generation efficiency and methane used in the catalytic burner	36
Figure 25. Simplified process flow diagram of the BioZEG plant including additional BOP [21].	39
Figure 26. Parametric tables for Figure 16 and 17	43
Figure 27. Parametric tables for Figure 18 and 19	44
Figure 28. Parametric tables for Figure 20 and 21	44
Figure 29. Parametric tables for Figure 22	45

## List of tables

Table 1. An ICE table for reaction (1) .....	12
Table 2. ICE table for the reformer where $x_1$ , $x_2$ and $x_3$ represent the change in steam methane reformation (Eq. (1)), water gas shift (Eq. (2)) and carbonation (Eq. (3)) respectively .....	20
Table 3. ICE-table for reactions taking place in the regenerator. Where $x_1$ and $x_2$ represent the change in steam methane reformation (Eq. (4)) and (Eq. (4)) reverse water gas shift (Eq. (2)) respectively .....	21
Table 4. ICE table for the SOFC where $x_1$ and $x_2$ represent the change in steam methane reformation and (Eq. (1)) water gas shift (Eq. (2)) respectively .....	23
Table 5. ZEG power 50 kW plant data for comparison of EES model .....	27
Table 6. ZEG Power 400 kW plant data for comparison of EES model .....	28

## Abbreviations

<i>Acronym</i>	<i>Definition</i>
ZEG	Zero Emission Gas
CCS	Carbon Capture and Storage
IPCC	Intergovernmental Panel on Climate Change
SER	Sorption-Enhanced Reformer
SOFC	Solid Oxide Fuel Cell
IFE	Institute for Energy Technology
EES	Engineering Equation Solver
BoP	Balance of Plant
SMR	Steam Methane Reforming
WGS	Water Gas Shift
LHV	Lower Heating Value
FU	Fuel Utilization
OU	Oxygen Utilization
ICE	Initial, Change and Equilibrium
SATP	Standard Ambient Temperature and Pressure

# Symbols

## Nomenclature

$\Delta H^{\circ}_f$	Heat of formation at 273°K and 1 atm [kJ/mol]
$V_{Nernst}$	Nernst voltage [V]
$E^0$	Open-circuit voltage [V]
$V$	Operational voltage [V]
$\eta_{act}, \eta_{ohm}, \eta_{conc}$	Voltage losses [V]
$R$	Proportionality constant
$F$	Faradays Constant
$P_i$	Partial pressure of substance $i$ [atm]
$T$	Temperature [K]
$I$	Current [A]
$\dot{n}$	Molar Flow [mol/s]
$K_p$	Equilibrium constant
$d\dot{E}$	Change of energy [J/s]
$\dot{Q}$	Heat [J/s]
$\dot{W}$	Work [J/s]
$\dot{m}$	Mass flow [kg/s]
$C_p$	Heat capacity [J/kg-K]
$\eta$	Efficiency



# 1 Introduction

## 1.1 Background and motivation

For decades, human kind has depended on fossil fuels. This dependence has set a need for decreasing greenhouse gas emissions according to the intergovernmental panel on climate change (IPCC) [1]. Even though the incline in greenhouse gas emissions are an imminent threat to the climate changes, our dependence on fossil fuels is still rising. A different report accomplished by IPCC states that Carbon Capture and Storage (CCS) technology can be a key in order to minimize overall environmental impacts [2]. CO<sub>2</sub> capture technologies are separated into different types of systems; one of them is pre-combustion technology, which allows production of hydrogen with CO<sub>2</sub> capture from biomass or fossil fuels. The hydrogen produced from pre-combustion technologies can be utilized in various applications, such as transport and electricity generation. Because hydrogen is an important energy carrier it has the potential of being a key to reducing current greenhouse gas emissions. The energy that hydrogen carries can be utilized in fuel cells. Fuel cell is a general term for electrochemical cells that transforms the combustion energy of hydrogen to generate electrical power.

The Zero Emission Gas (ZEG<sup>®</sup>) technology is an innovative technology that allows co-production of hydrogen and electricity with integrated CO<sub>2</sub> capture. The technology can utilize hydrocarbon gases both from fossil or renewable sources at very high efficiency (>75%) and can contribute to a CO<sub>2</sub> emission free future. The technology combines two core technologies; Sorption-Enhanced Reforming (SER) and Solid Oxide Fuel Cell (SOFC) [3].

The company ZEG Power is developing the technology with the purpose to commercialize ZEG plants. A small scale demonstration plant of 50 kW (30 kW hydrogen + 20 kW electricity) was constructed and operated at HyNor Lillestrom, a hydrogen and fuel cell technology test centre near Oslo, Norway [3, 4]. Results from tests and optimisation are used for scale-up of the technology to a 400 kW scale power plant (200 kW hydrogen + 200 kW electricity). Process simulation of the ZEG-technology has been carried out in the framework of different projects [3, 5]. Predictive simulation was done in order to optimize the process, exploit the technology's full potential and to build a base for design, pre-engineering and cost estimation of ZEG plants.

In particular, detailed predictive simulation of the SER process was carried out by Institute for Energy Technology (IFE) with extensive modulation, considering both thermodynamics, kinetics and fluid dynamics [6]. The results of the simulations were used in the framework of two projects, BioZEG and ZEG400 for the concept design of ZEG components respectively in a 50 kW; the BioZEG plant, and a 400 kW scale plant.

The predictive simulations carried out so far on the SER and the SOFC- processes have been experimentally validated and have shown to predict the behaviour of the technology with small errors. The simulations are however limited by the use of specific engineering parameters and several iteration on different simulating platforms (HYSYS, MatLab) every time plant inputs and boundary condition are changed. The lack of a simplified tool including both the SER and the SOFC-process for initial studies of different plant configurations was identified as a useful improvement for the evaluation of different technology applications.

## 1.2 Goals

The main goal of the present thesis was to create a simplified zero-dimensional model for the ZEG-technology through energy balance calculations. For the model, only thermodynamics and chemical equilibrium were considered. The results generated from the simulation were compared with previous simulations, in order to validate the quality of the model created in this thesis, in particular:

- The zero dimensional simulation of the ZEG-technology was done with the software *engineering equation solver* (EES).
- The simulation involved only thermodynamics of the SER and SOFC-processes and for part of the high temperature section involved in the process. Balance of plant (BoP) such as high temperature heat exchangers for heat recirculation and other auxiliaries, were not included in the study as the main purpose is to obtain a tool for comparison and sensitivity analysis and not an accurate estimation of the performance of a ZEG plant

## 2. The ZEG-technology

### 2.1 Introduction

The ZEG - technology is a hybrid technology for co-production of electricity and hydrogen from hydrocarbon fuels, with integrated CO<sub>2</sub> capture. The basic technologies in the ZEG-concept are a SER for hydrogen production and a SOFC for electricity production. Surplus heat from the SOFC-module is supplied to the SER reactor system, which reforms incoming hydrocarbon fuel to hydrogen. Simultaneously the SER-system yields a separate stream of CO<sub>2</sub>. The close to pure hydrogen is fed to the SOFC, where electric power is produced. The hydrogen rich SOFC exhaust is then after purification ready for a wide range of industrial applications. The ZEG-technology is able to produce hydrogen and electricity, at very high efficiency; potentially more than 75% is possible, including carbon capture [3], [7]. Close thermal integration of the two basic technologies is necessary in order to obtain a high total efficiency [5].

The ZEG -technology is flexible in being able to co-generate power and hydrogen, in addition both core technologies can be used for standalone hydrogen (SER) end electricity production (SOFC). A simplified schematic of the ZEG-technology is shown in Figure 1.

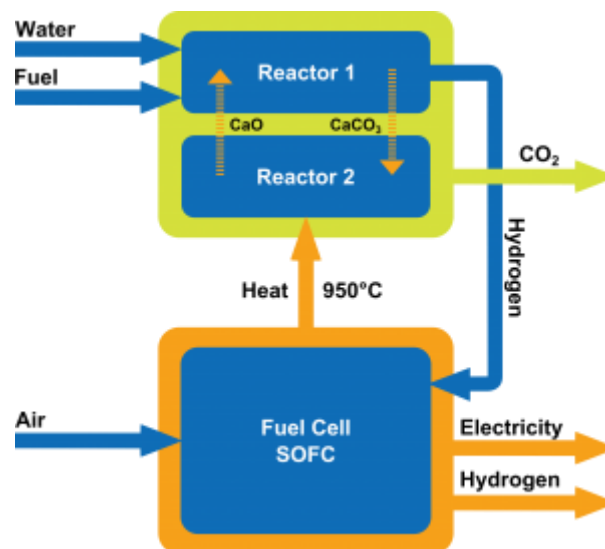


Figure 1. Simplified scheme of the ZEG-technology [3].



## 2.2 Sorption-Enhanced Reforming (SER)

SER is an innovative reforming technology for hydrogen production that allows CO<sub>2</sub> capture at high temperature [5, 8]. It combines reforming, water gas shift and CO<sub>2</sub> capture in the same reactor (reformer) providing a process intensification with hydrogen production in one single step. This is made possible by the introduction of a high temperature solid CO<sub>2</sub> sorbent, mixed together with the reforming catalyst, in the reaction. The CO<sub>2</sub> captured as a solid carbonate is released by increasing the temperature in a second reactor, the regenerator. In this step, heat has to be provided via a high temperature heat exchanger or via oxy-combustion. The key advantages of adding the SER are [8]:

- Overall process simplification and intensification
- No need for water gas shift reactors and catalysts
- Higher hydrogen yield compared to conventional SMR
- CO<sub>2</sub> is simultaneously separated in the reaction and nearly pure CO<sub>2</sub> is obtained by regenerating the CO<sub>2</sub>-sorbent using high temperature heat.

The SER reformer and the regenerator are interconnected by a solid loop to allow CO<sub>2</sub> capture and regeneration of solids in continuous mode. The solids in the SER mainly consist of a CO<sub>2</sub> sorbent (usually calcined dolomite) and a catalyst for the reforming reaction. The calcined dolomite is a complex molecule that can be derived as CaO in addition to MgO [8]. A schematic of how the SER works is shown in Figure 2.

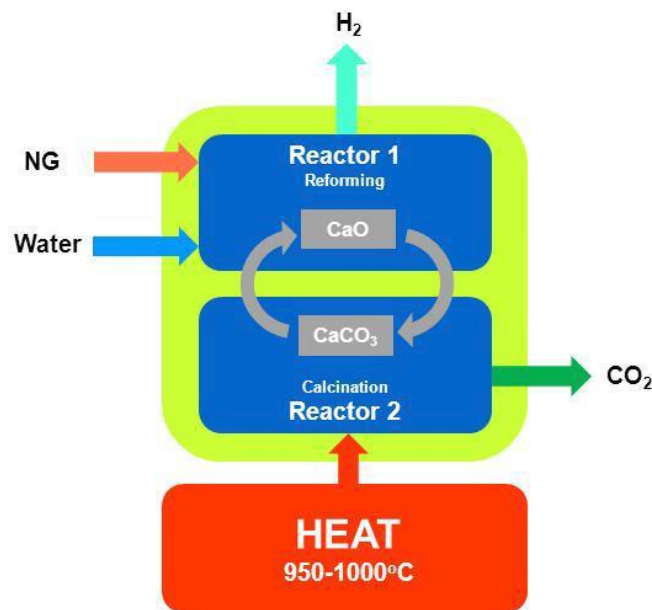
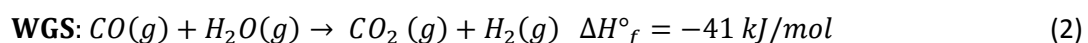
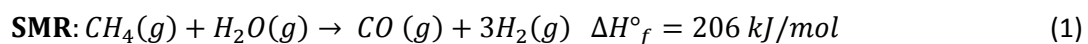
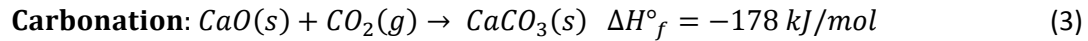


Figure 2. Simplified scheme of the SER system [4].

### 2.2.1 Reformer

In the reformer, the presence of the reforming catalyst and the CO<sub>2</sub> sorbent allows the simultaneous combination of three reactions: Steam Methane Reforming (SMR), Water Gas Shift (WGS) and carbonation, shown respectively in the equations 1, 2 and 3 [8, 9].





Conventional reformers involve SMR without carbonation bringing to a hydrogen yield of around 75% (dry-basis) at temperatures above 650°C. The simultaneous removal of CO<sub>2</sub> in the SER moves the thermodynamic equilibrium towards higher hydrogen production yield at lower temperatures, and hydrogen concentrations up to 98 vol% (dry basis) can be obtained in the temperature range of 550 – 650°C (Figure 3) [6].

The partially carbonated calcined dolomite generated in the reformer is transported through the solid loop to the regenerator. Both homogeneous and heterogeneous equilibria are involved in the reformer.

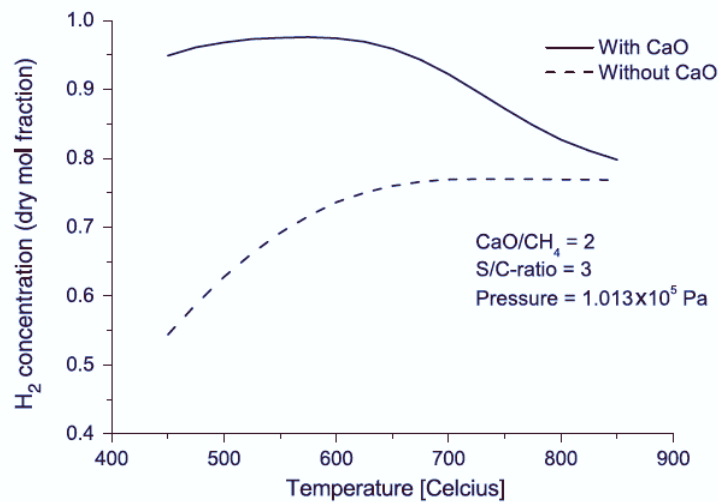
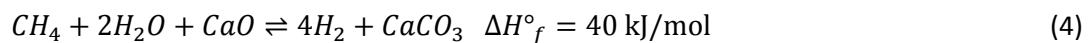


Figure 3. Thermodynamic equilibrium for conventional SMR and SER [6].

The reformer undergoes change of state with respect to reactions. As the carbonation reaction is exothermic, part of the heat needed for reforming is provided by this reaction. The total reaction is thought to be slightly endothermic as shown in the equation for the total reaction:

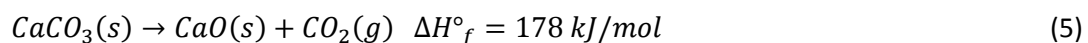


where reaction (4) is a summation of SMR (1), WGS (2) and carbonation (3) reactions.

The solid substances entering the system are compensating the heat need of the regenerator [6], making the reformer nearly auto-thermal.

### 2.2.2 Regenerator

In the regenerator, the formed carbonate undergoes calcination (regeneration) as shown in the following equation.



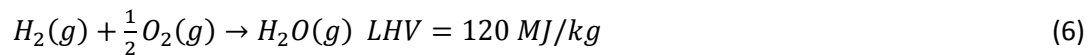
This reaction takes place at a temperature of 850°C, and is considered to have and complete evolution towards the products. To prevent the catalyst from oxidizing, hydrogen and water are fed to the regenerator. The regenerated calcined dolomite is transported to the reformer for reuse. Since the reaction of calcination is an endothermic reaction, the reaction requires heat. In the ZEG-technology, heat is provided by a SOFC using a heat exchanger immersed in

the regenerator. If necessary the SOFC transfers high quality waste heat to a catalytic burner for temperature boost up, and consequently to the regenerator via the heat exchanger [6]. In a configuration for standalone hydrogen production, solid regeneration is performed by use of the catalytic burner with pre-heated air and fuel, without the support of a SOFC.

### 2.3 Solid Oxide Fuel Cell (SOFC)

The theory in the subsequent section is largely based on the book *Solid oxide fuel cell technology* [10] unless other references are presented.

Fuel cells use hydrogen as fuel to produce electricity. The process can be described as hydrogen combining with oxygen to produce water as shown in the following equation:



where the *LHV* is the lower heating value for hydrogen combustion.

Reaction (6) can be separated into two reactions, cathodic and anodic. The cathode is the positive electrode where a chemical reduction takes place, whilst the anode is the negative electrode where oxidation occurs. The anodic and cathodic reactions for the SOFC can be written as follow[11]:



Different type of fuel cells have been developed for different purposes (transport, mobile, stationary etc.), each one characterized mainly by the type of electrolyte and by the operating temperature. Between high temperature fuel cells, SOFC with planar configuration are well know for being an optimal option for stationary applications. This type of fuel cell is the one used in the present ZEG-technology. The SOFC is characterized by a solid electrolyte and operates at a high temperature (600-1000°C). Fuel cells usually transfer the hydrogen through an electrolyte. The SOFC is the only fuel cell that transfers the oxygen through the electrolyte so that water is produced at the anode as shown in Figure 4. The electrolyte is usually yttrium stabilized zirconium, which is a  $ZrO_2$  doped with  $Y_2O_3$ , which leaves oxygen vacancies in the zirconia structure as shown in Figure 5. This allows the oxygen ions to migrate through the electrolyte.

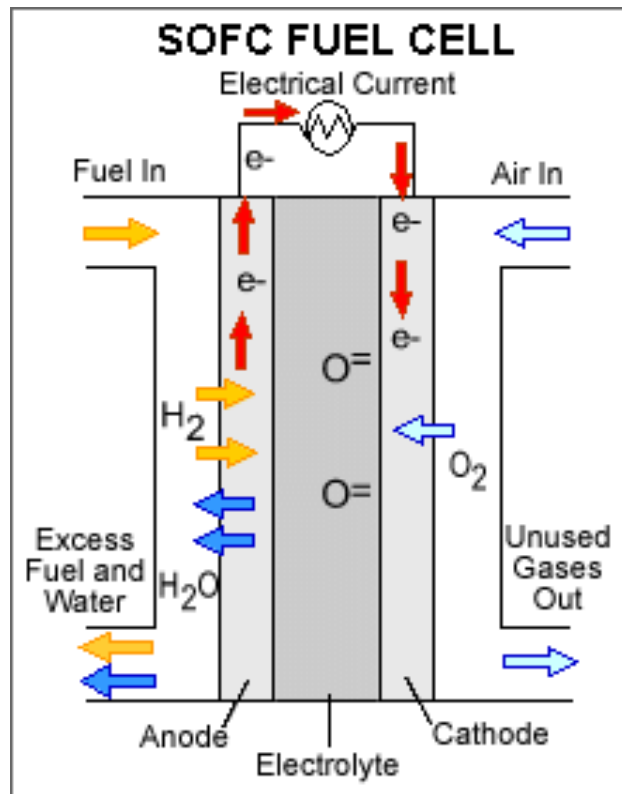


Figure 4. General description of SOFC function [12].

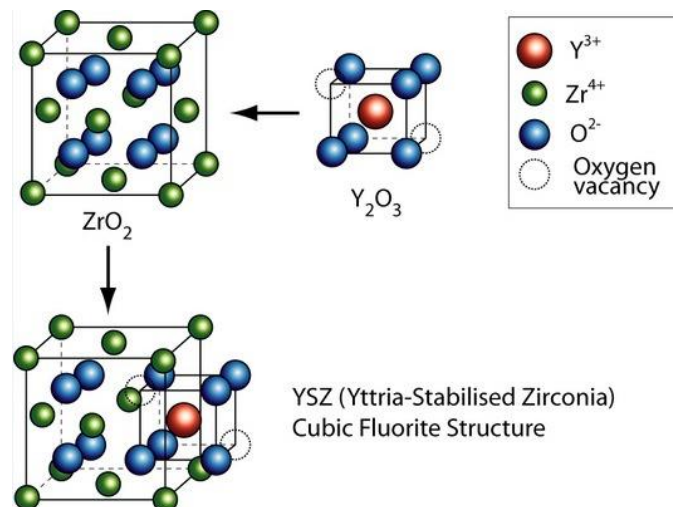


Figure 5. Yttrium-Stabilized Zirconia molecule 3-D structure [13].

The anode of the SOFC is normally Ni-ZrO<sub>2</sub> cermet, which is a mixture between ceramics and metal, and the cathode is Sr-doped LaMnO<sub>3</sub>. In basic, the disadvantage of SOFC are related to the possible breakage of the anode under mechanical stress at high temperature [10]. The interconnection of a SOFC stack is shown in Figure 6. The key advantages of the SOFC are [10]:

- High efficiency generation of power
- Chemical energy in fossil fuels can be directly converted to generate power
- Produces high-quality waste heat

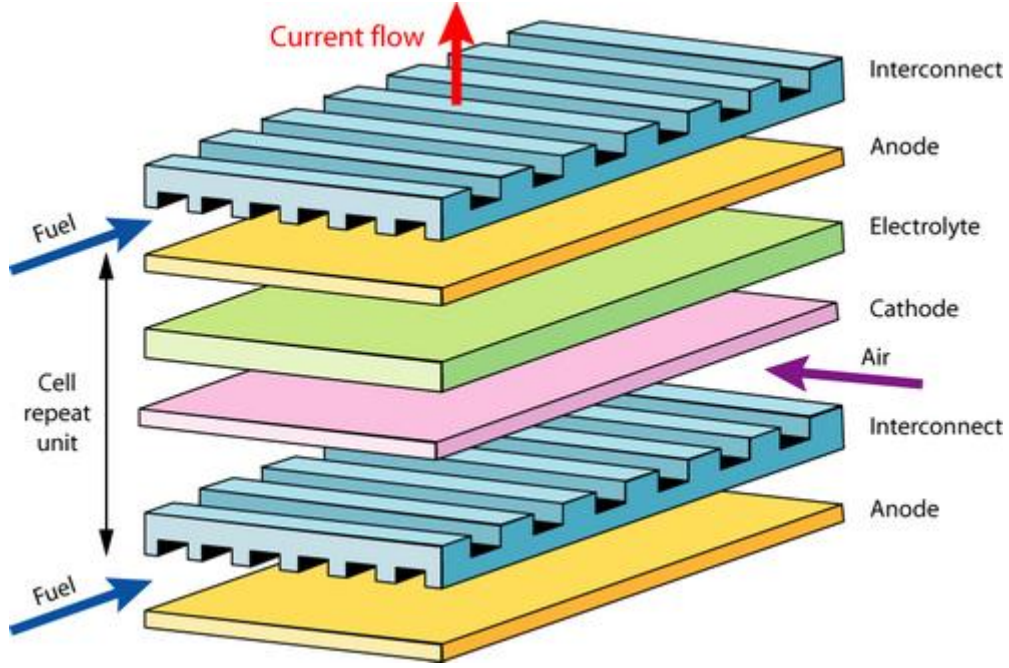


Figure 6. Stack configuration of a planar SOFC [12]

The Nernst equation is used to define the theoretical open circuit voltage of a fuel cell, also known as the Nernst voltage. The Nernst voltage takes into account the losses of chemical mixture and can be shown as [14]:

$$V_{Nernst} = E^0 + \frac{RT}{2F} \ln\left(\frac{P_{H_2} P_{O_2}^{0.5}}{P_{H_2O}}\right) \quad (9)$$

where  $P_{H_2}$ ,  $P_{O_2}$  and  $P_{H_2O}$  is the partial pressure of hydrogen, oxygen and water, and  $F$  is the Faraday constant. The  $E^0$  is the reversible cell voltage. The reversible cell voltage,  $E^0$ , is a theoretical value of the voltage only considering the Gibbs free energy of the system and can be expressed by the following formula [15]:

$$E^0 = 1,253 - 2,4516 \cdot 10^{-4}T \text{ [V]} \quad (10)$$

where  $T$  is the operational temperature at which the fuel cell is operating.

The losses that occur under operating conditions can be separated into three parts, activation, ohmic and concentration losses. The activation losses is associated to the splitting of oxygen into an electron and a proton upon traveling through the electrolyte and combining with hydrogen. The activation losses is dependent on the operational temperature [11]. The ohmic losses is related to the electron flow through a surface, which is common in every electronic device. This is dependent on the specific resistance of the surface and the flow rate of the charged particle that the ion is travelling through a specific surface. The concentration loss is related to the gas mixture and the rate at which the fuel is consumed. The three operational losses are illustrated in Figure 7. The three abovementioned losses yields the operational voltage, which is expressed as [15]:

$$V = V_{Nernst} - (\eta_{act} + \eta_{ohm} + \eta_{conc}) \quad (11)$$

where  $\eta_{act}$ ,  $\eta_{ohm}$  and  $\eta_{conc}$  is the activation, ohmic and concentration losses, respectively.

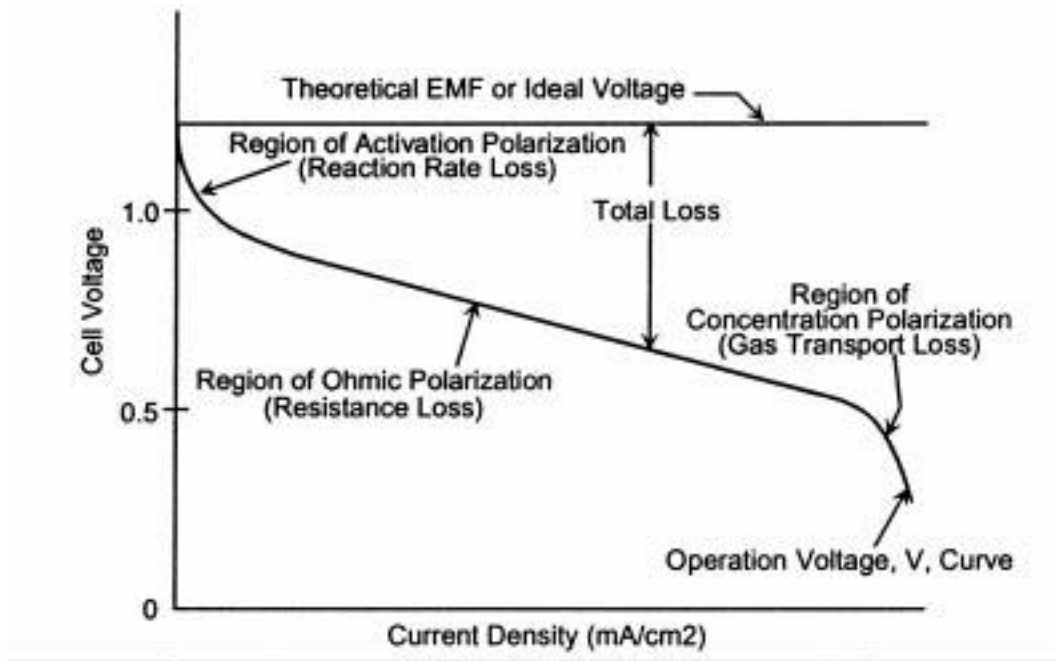


Figure 7. The operational losses through an electrolyte when increasing the current density [11].

The production of power is dependent on how much hydrogen is utilized at the anode, which is defined by the Fuel Utilization (FU) and is given by:

$$FU = \frac{\dot{n}_{utilized\ fuel}}{\dot{n}_{available\ fuel}} \quad (12)$$

The FU directly influences the amount of oxygen needed in the cell, since one mole of hydrogen reacts with half a mole of oxygen as shown in reaction (6). The cathodic inlet airflow is defined by the Oxygen Utilization (OU) and can be written as:

$$OU = \frac{\dot{n}_{utilized\ oxygen}}{\dot{n}_{available\ oxygen}} \quad (13)$$

The current of one cell can be calculated by the following formula [16]:

$$I = 2F \cdot \dot{n}_{utilized\ fuel} \cdot FU \quad (14)$$

where  $\dot{n}_{utilized\ fuel}$  is the molar flow of hydrogen utilized by one cell (anode, cathode and electrolyte).

The power generated by a single fuel cell is equal to the real voltage of the cell (Eq. (11)) multiplied by the current generated by one cell (Eq. (14)):

$$P = V \cdot I \quad (15)$$



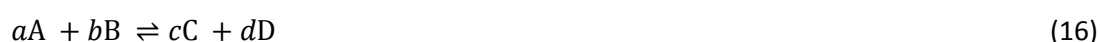
### 3. Simulation

#### 3.1 Model theory

In this section, the theory used for the simulation of the ZEG-technology is generally described.

##### 3.1.1 Equilibrium

A Chemical Equilibrium is defined as “when the rates of forward and reverse reaction are equal and the concentration of the reactants and products no longer change with time” [17]. The reactions are restricted to the amount of substances that can involve in a forward reaction. The reason is that each substance involved in the reaction have a concentration (mol/L) which inhibits the reaction from moving forward (to the right). Equilibrium of a general reaction can be written as [17]:



in which  $a$ ,  $b$ ,  $c$  and  $d$  can be viewed as the stoichiometric coefficients for A, B, C and D that are the reacting gaseous substances. The substances on the right side of the equilibrium are the reactants and the substances on the left side of the equilibrium are the products. One can illustrate an equilibrium going from an initial state to a state where no forward or backward reactions are changing with time in Figure 8.

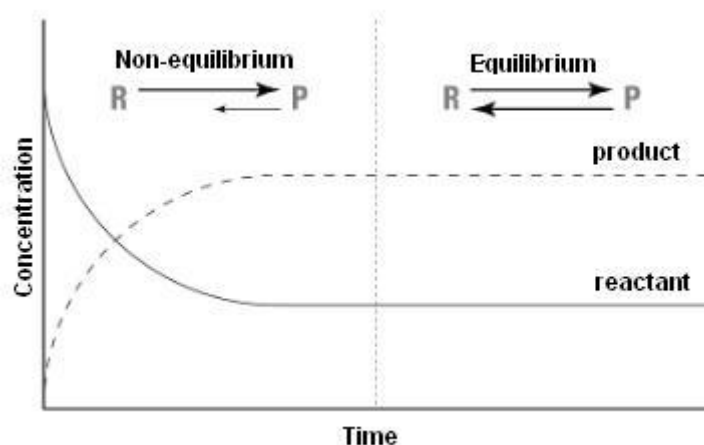


Figure 8. Graphic illustration of equilibrium[18].

The change in initial amount of substances can be decided by the equilibrium constant, which defines the forward or backward rate of the reaction. When considering an equilibrium reaction in which the substances are gaseous and temperature is constant, the equilibrium constant can be calculated as [17]:

$$K_p = \frac{P_C^c P_D^d}{P_A^a P_B^b} \quad (17)$$

where  $P_A$ ,  $P_B$ ,  $P_C$ ,  $P_D$  are the final partial pressure of substance A, B, C and D participating in the reaction. Through the ideal gas law [17]:

$$PV = nRT \quad (18)$$



where  $P$  is pressure,  $V$  is volume,  $n$  is the amount of mole,  $R$  is the proportionality constant and  $T$  is the temperature. We can re-formulate Eq. (17) as:

$$K_P = \frac{n_C^c \cdot n_D^d}{n_A^a \cdot n_B^b} \cdot \frac{P_{tot}^{(c+d)-(a+b)}}{n_{tot}^{(c+d)-(a+b)}} \quad (19)$$

assuming that the temperature  $T$  and volume  $V$  is constant. From Eq. (19) one can find the amount of moles involved in the forward reaction also known as the change in reaction. The change ( $x$ ) of a reaction is decided by the initial amount (mol) of each substance (A, B, C and D) participating in the reaction:

$$K_P = \frac{(n_{C,initial}+x)^c \cdot (n_{D,initial}+x)^d}{(n_{A,initial}-x)^a \cdot (n_{B,initial}-x)^b} \cdot \frac{P_{tot}^{(c+d)-(a+b)}}{n_{tot}^{(c+d)-(a+b)}} \quad (20)$$

where  $n_{A,initial}$ ,  $n_{C,initial}$ ,  $n_{D,initial}$ ,  $n_{D,initial}$  are the initial amount of moles in the equilibrium reaction (1) and  $x$  is the amount of moles that change in the equilibrium reaction.

An equilibrium can be visualized by using a table for the Initial, Change and Equilibrium (ICE) state of each substance when given an equilibrium constant. An example for reaction (16) is given in Table 1.

Table 1. An ICE table for reaction (1)

Substance:	Initial	Change	Equilibrium
A	$n_{A,initial}$	$-x$	$n_{A,initial} - x$
B	$n_{B,initial}$	$-x$	$n_{B,initial} - x$
C	$n_{C,initial}$	$+x$	$n_{C,initial} + x$
D	$n_{D,initial}$	$+x$	$n_{D,initial} + x$
Total	$n_{A,initial} + n_{B,initial}$ $+ n_{C,initial}$ $+ n_{D,initial}$	0	$n_{A,initial} + n_{B,initial}$ $+ n_{C,initial}$ $+ n_{D,initial}$

### 3.1.2 First law of thermodynamics

The first law of thermodynamics states that “for steady flow, the external work done on any system plus the thermal energy transferred into or out of the system is equal to the change of energy of the system” [19]. The change of energy of a control volume (involving a mass flow) can be formulated as [14]:

$$d\dot{E} = \delta\dot{Q} - \delta\dot{W} \text{ [kW]} \quad (21)$$

where  $\delta\dot{Q}$  is the transferred heat into or out of the system and  $\delta\dot{W}$  is the work done or applied on the system. The work applied on a system by a control volume is defined by the rate of flow work [14]:

$$\dot{W} = P\dot{V} \text{ [kW]} \quad (22)$$

where  $P$  is pressure and  $\dot{V}$  is the volumetric flow. The heat transferred into or out of a system by a substance can be written as the following equation given that the pressure is constant [14]:

$$\dot{Q} = \dot{m} \cdot C_p(T) \cdot (T_2 - T_1) \quad [\text{kW}] \quad (23)$$

where  $\dot{m}$  is the mass of the substance and  $T_2$  is the temperature to which the substance has been heated from  $T_1$ . The constant pressure specific heat capacity ( $C_p(T)$ ) is defined as the amount of heat required to rise the temperature of one kilogram of a substance from a temperature ( $T_1$ ) to a temperature of  $T_2$  at constant pressure. The heat capacity of a substance typically follows the form [10]:

$$C_p(T) = a + b \cdot T + c \cdot T^2 + d \cdot T^3 + e \cdot T^{-2} \quad \left[ \frac{\text{kJ}}{\text{kg} \cdot \text{K}} \right] \quad (24)$$

where  $a, b, c, d, e$  are coefficients of the substance that is being considered.

When considering a reacting system in which the pressure is assumed constant and no work is done, Eq. 21 can be rewritten as [14]:

$$\dot{Q}_{In} = \dot{Q}_{Out} + \dot{H}_f \quad (25)$$

where  $\dot{Q}_{In}$  is the heat of the substances going into a system,  $\dot{H}_f$  is the enthalpy of formation at a given temperature relative to a reference temperature and  $\dot{Q}_{Out}$  is the heat of the substances going out.

For the heat of a substance ( $i$ ) presumed to be going in or out of a system at a temperature of  $T_1$ , one can apply the average heat capacity method [20]:

$$\dot{Q}_i = \dot{m}_i \cdot C_{p,avg} \cdot (T_1 - T_0) \quad [\text{kW}] \quad (26)$$

where the  $\dot{m}_i$  is the mass flow of the substance being considered,  $T_1$  is the temperature at which the substance is being considered,  $T_0$  is the relative reference temperature of 25°C. The  $C_{p,avg}$  is the average heat capacity that is given by the average temperature of  $T_0$  and  $T_1$ .

The first law of thermodynamics Eq. (21) is referred to as energy balance analysis in this thesis.

### 3.2 Engineering equation solver (EES)

The following section and its theory is from *EES: Engineering equation solver for Microsoft Windows Operating Systems* [21] which is a user manual for the software.

Unlike other programming tools that only allow assignments, EES allows one to solve equations, which is a relationship between variables. The software does not consider whether variables are on the left or the right side of the equal sign. EES organizes equations into subgroups of equations that need simultaneous solution. These subgroups are called blocks and EES solves these using a built-in iterative process. Though EES may find multiple solutions to a variable it will choose the closest solution to the set guess value, which is pre-set to the value of one. Guess values will be described more thoroughly in subchapter 3.2.1.

EES has built in thermodynamic functions as enthalpy, specific heat etc. for several ideal and real substances. EES also has functions for conversion between units and temperature. The software identifies most known units as kJ, kg, kW etc. EES also has a unit checking function

so that inconsistencies regarding the units are avoided. The user has the option to set the units in which EES operates.

EES allows the user to make diagrams. The diagram window allows the user to make user-friendly graphical program. This allows a user to interact with EES without having to modify the equations. An example of a typical diagram is shown in Figure 9.

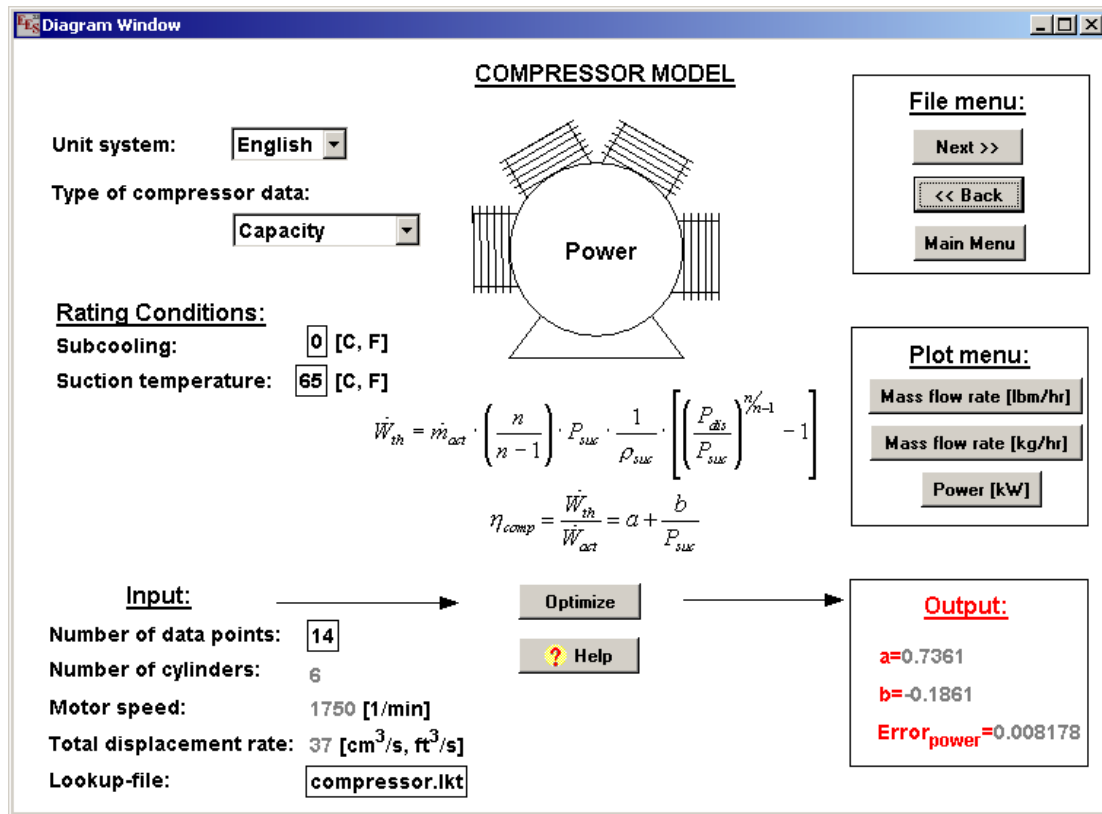


Figure 9. Example of a diagram created in EES [21].

When making a model some users may prefer to study their dependent variable upon changing their independent variable. This can be accomplished in parametric tables, which can be generated in EES. It is also possible to make plots of these generated parametric tables. An example of a parametric table and plots made for the interval  $1 \leq x \leq 10$  of the linear function  $y = 2 \cdot x$  is shown in Figure 10.

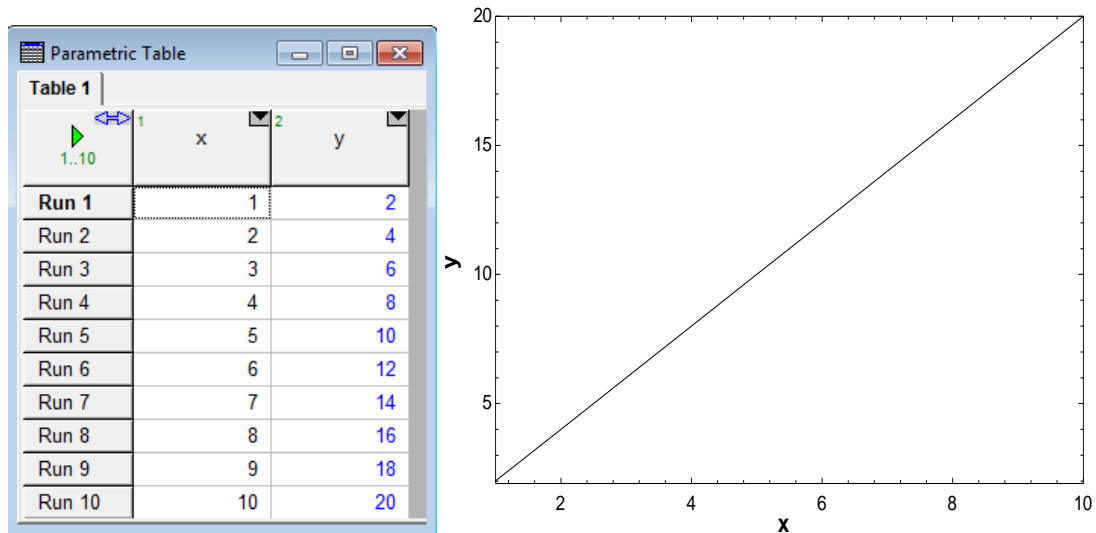


Figure 10. Example of a parametric table and plot for the function  $y = 2*x$

### 3.2.1 Guess value, upper and lower limits

Guess values, upper and lower limits are useful when an answer to a non-linear algebraic function is not satisfactory or logical. If a general equation is to be solved within certain limits, one can set the upper and lower limit for the unknown that is being evaluated. When you still have multiple solutions within set domain, one can utilize the guess value function of EES. The guess value function finds a solution near a set guess value by evaluating the residual of the variable equal to zero. EES uses Newton's method to evaluate a solution for a non-linear solution. Newton's method can be shown as the following formula:

$$x_{i+1} = x_i - \frac{f(x_i)}{\left(\frac{df}{dx}\right)_{x=x_i}} \quad (27)$$

where we begin with a guess value (estimate)  $x_i$  and evaluate the residual  $f(x_i)$  over the derivative  $\left(\frac{df}{dx}\right)_{x=x_i}$  with respect to  $x_i$ . This is done with iteratively until EES finds the root of  $f(x_i)$ .

### 3.1.2 Built-in functions

EES has several built-in functions that are useful to engineering application. Amongst these, there are mathematical, heat transfer & fluid flow, mechanical design and thermodynamic properties. The functions can be called in the equation window. An example for calling the specific heat capacity of methane is given in Figure 11. As one can see from Figure 11, the user must implement conditions for the function being called.

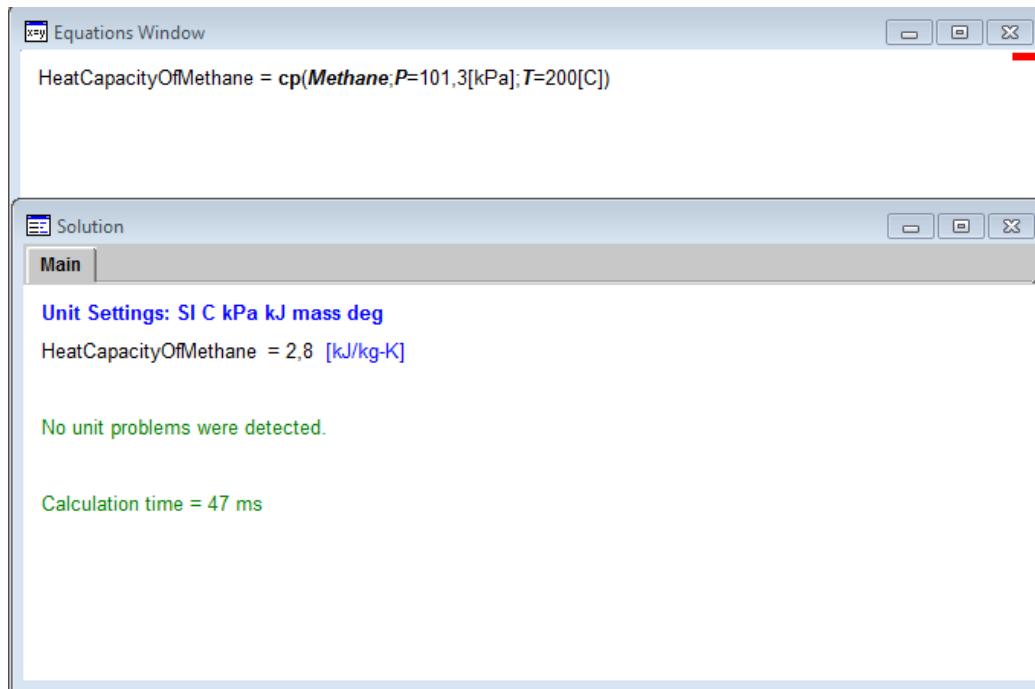


Figure 11. Example of calling the heat capacity of a substance in EES

### 3.3 Previous work

The simulation of the SER process in combination with SOFC has been carried out by ZEG Power in cooperation with IFE [3, 5, 6]. The SER has been modelled for bubbling fluidized beds [6]. This model combine kinetics (for both reforming and carbonation), thermodynamics and hydrodynamics.

For initial concept studies and optimization of the ZEG-technology, this model is far too complicated and combination with process simulation of a full ZEG plant is needed to save time. For this purpose, similar simulation of both the SER and the SOFC were developed by both IFE and ZEG in EES. The models give a complete mass and energy balance, and has helped to identify critical parts to improve efficiencies of the process. However, these models are either incomplete (only SER is considered) or are limited by the use of specific engineering parameters and several iteration on different simulating platforms (HYSYS, MatLab) are needed every time the plant inputs and boundary condition are changed

When studying alternative plant configurations for the formulation of research proposal and for patenting purposes, a simplified model of a full ZEG plant – from gas feed to electricity and hydrogen production is thus needed. The results from the previous simulation done by IFE and ZEG, and in particular, the work carried out during the BioZEG and ZEG400 projects, were used for comparison and validation.

### 3.4 Simulation of the ZEG-technology

The simulation of the ZEG-technology was done considering a zero dimensional model. Fluid dynamic was not taken into account in the model. For the control volume in which the zero dimensional model is to be considered the following systems were considered:

- Reformer
- Regenerator
- SOFC
- Catalytic burner

The developed model is based on a configuration of the ZEG-technology including a catalytic burner, in addition to waste heat from the SOFC for regeneration of sorbent. This choice is related to the fact that commercial SOFCs that can be utilized in ZEG-technology are normally operating at temperatures of maximum 850°C. Therefore, an catalytic burner is implemented to increase the temperature for regeneration of sorbent up to around 1050°C. When the process is used for stand-alone hydrogen production, the power of the SOFC is set to zero and the catalytic burner is fed with pre-heated air (heat is recirculated from the regenerator exhaust) and fresh fuel. Figure 12 illustrated the basic simulation design of the system.

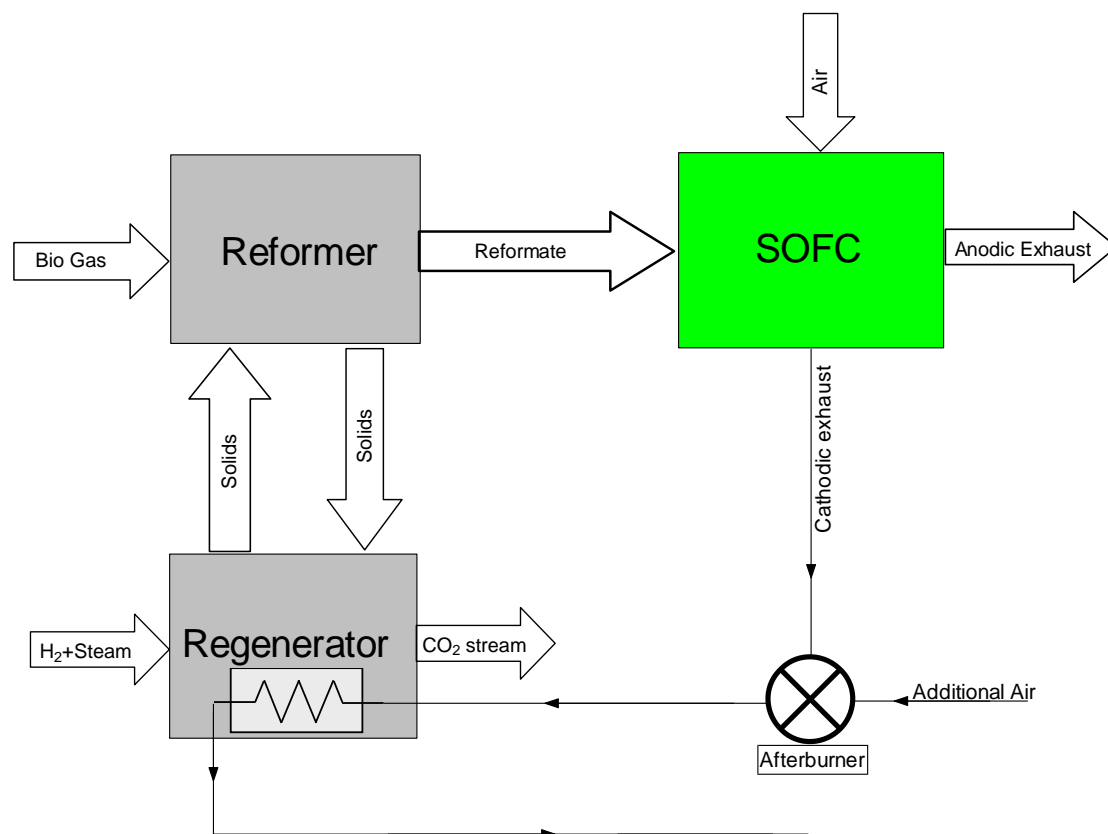


Figure 12. Basic model design for the chose ZEG configuration

The assumption that were made for the whole model was:

- Steady-state
- System of reference is Standard Ambient Temperature and Pressure (SATP)
  - 25°C
  - 1 atm

The general approach for the chosen ZEG-configuration was to consider a control surface for which we consider energy balance. The number of unknown equations for the control surface is the same as the number of independent equations. This gives the results for the system.

For the same model, we also know the chemical reactions and presume to know the losses for each system being considered. Therefore, one can use Eq. (25) on each of the systems as illustrated in Figure. 13.

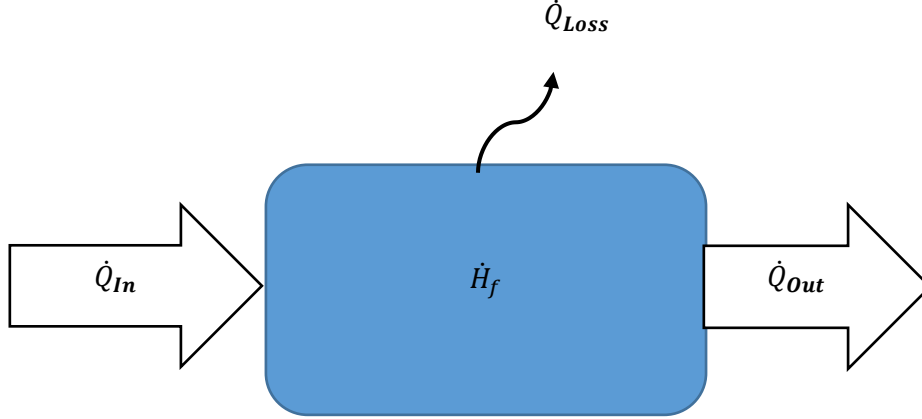


Figure 13. Box surface of the simulation model

When solving the equilibrium of the three systems (regenerator, reformer and SOFC) Eq. (2) is used to solve multiple equilibriums simultaneously. ICE-tables as shown in Table 1 are developed in order to illustrate the change in equilibrium. The equations created by this approach generate multiple variable equation sets. This is was done in EES by setting guess values for each substance.

For the system, two types of efficiencies are considered, standalone and co-generation. The results from the two configurations and in particular the efficiencies in each case are relevant to understand the model. Efficiency can be described as energy output with respect to energy input. Since methane is fed to the catalytic burner for temperature boost up, this has to be considered as part of the energy input. The efficiency for the standalone generation is given by:

$$\eta_{\text{Stnadalone}} = \frac{\dot{m}_{H_2, \text{out, reformer}} \cdot LHV_{H_2}}{(\dot{m}_{CH_4, \text{in, reformer}} + \dot{m}_{CH_4, \text{in, burner}}) \cdot LHV_{CH_4}} \quad (28)$$

where  $\dot{m}_{H_2, \text{out, reformer}}$  is the hydrogen mass flow out of the reformer,  $LHV_{H_2}$  is the lower heating value of hydrogen,  $\dot{m}_{CH_4, \text{in, reformer}}$  is the methane mass flow into the reformer,  $\dot{m}_{CH_4, \text{in, burner}}$  is the methane mass flow into the catalytic burner and  $LHV_{CH_4}$  is the lower heating value of methane.

The efficiency for the co-generation of hydrogen and electricity is given by:

$$\eta_{\text{Co-generation}} = \frac{(\dot{m}_{H_2, \text{out, reformer}} \cdot LHV_{H_2} + P_{el})}{(\dot{m}_{CH_4, \text{in, reformer}} + \dot{m}_{CH_4, \text{in, burner}}) \cdot LHV_{CH_4}} \quad (29)$$

where  $P_{el}$  is the electric power generated by the SOFC.

The full set of equations used for simulating the ZEG-technology can be found in Appendix B.

### 3.4.1 Sorption-Enhanced reforming

The simulation setup for the SER can be illustrated as shown in Figure 14. The reformer and regenerator were simulated as separate control surfaces and their only interactions were through the solid-state substances (calcined dolomite and catalyst). As the model is considered in steady state, time dependence does not influence the equilibrium.

The simulation of the SER should provide useful output data for the user. The output data was set to result in heat needed for the regenerator, inlet temperature of the reformer and the composition of the substances leaving both the reformer and regenerator. Since the simulation was done in a zero dimensional space, loss through the pipes length was not considered.

The total energy balance for the SER was calculated through Eq. (25). The total heat loss in the reformer was set as a fraction of the heat going in the reformer:

$$\dot{Q}_{loss} = (\dot{Q}_{In}) * loss \quad 0 \leq loss \leq 1 \quad (30)$$

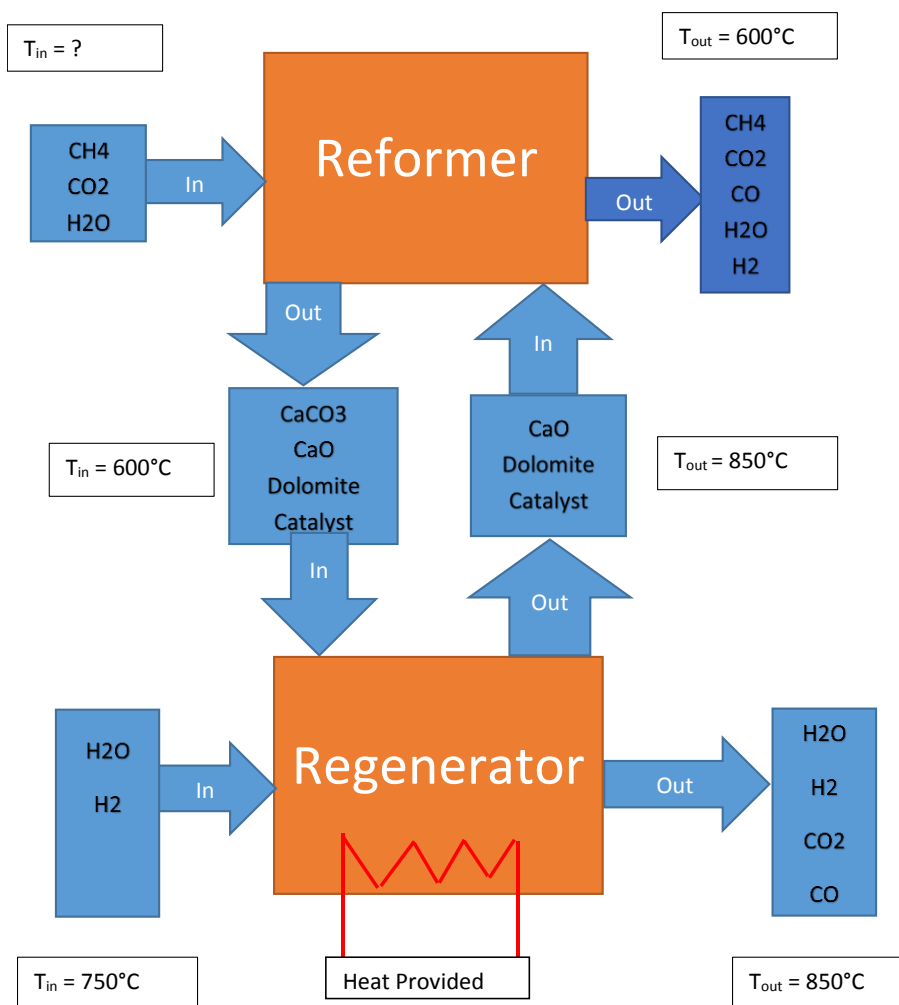


Figure 14. The control surface of the SER for the simulation in EES



### 3.4.1.1 Reformer

The simulation of the reformer was set to result in the inlet temperature of the gas. To approach this problem, substances that were involved in reactions were considered to have reached their chemical equilibrium before exiting the reformer. Equilibrium constants with temperature dependence ( $K_p$ ) was used in order to calculate the substance composition when exiting the reformer and the change in the reaction (Eq.(20)). The setup of the equilibrium (ICE-table) in the reformer is shown in Table 2. By implementing the ICE-table for the reformer on Eq. (20), the equilibrium equations for SMR, WGS and carbonation were as following:

$$K_{P,SR} = \frac{(x_1-x_2)(3x_1+x_2)^3}{(n_{CH_4,initial}-x_1)(n_{H_2O,initial}-x_1-x_2)} \cdot \frac{P_{tot}^2}{(n_{H_2O,initial}+n_{CH_4,initial}+n_{CO_2,initial}+2x_1-x_3)^2} \quad (31)$$

$$K_{P,WGS} = \frac{(n_{CO_2,initial}+x_2-x_3)(3x_1+x_2)}{(x_1-x_2)(n_{H_2O,initial}-x_1-x_2)} \quad (32)$$

$$K_{P,Carbonation} = \frac{1}{(n_{CO_2,initial}+x_2-x_3)} \cdot \frac{(n_{H_2O,initial}+n_{CH_4,initial}+n_{CO_2,initial}+2x_1-x_3)}{P_{tot}} \quad (33)$$

For the carbonation, the solid-state substances do not apply a partial pressure so they are not included in the equation.

Table 2. ICE table for the reformer where  $x_1$ ,  $x_2$  and  $x_3$  represent the change in steam methane reformation (Eq. (1)), water gas shift (Eq. (2)) and carbonation (Eq. (3)) respectively

<b>Substances</b>	<b>Initial (mol)</b>	<b>Change (mol)</b>	<b>Equilibrium (mol)</b>
$H_2$	0	$3x_1 + x_2$	$3x_1 + x_2$
$H_2O$	$n_{H_2O,initial}$	$-x_1-x_2$	$n_{H_2O,initial} - x_1-x_2$
$CH_4$	$n_{CH_4,initial}$	$-x_1$	$n_{CH_4,initial} - x_1$
$CO_2$	$n_{CO_2,initial}$	$x_2 - x_3$	$n_{CO_2,initial}+x_2 - x_3$
$CO$	0	$x_1 - x_2$	$x_1 - x_2$
$CaO$	$n_{CaO,initial}$	$-x_3$	$n_{CaO,initial}-x_3$
$CaCO_3$	0	$x_3$	$x_3$
Total	$n_{H_2O,initial}$ + $n_{CH_4,initial}$ + $n_{CO_2,initial}$	$2x_1 - x_3$	$n_{H_2O,initial}$ + $n_{CH_4,initial}$ + $n_{CO_2,initial} + 2x_1$ - $x_3$

Substances entering the reformer are considered to have reached the temperature of the reformer (600°C) before involving in an equilibrium. The composition (mol%) of the biogas entering the reformer is a value that is decided by the user. Steam entering the reformer is decided by a steam to carbon ratio (S/C-ratio). The inlet fuel is thought to be biogas which mainly consists of methane and carbon dioxide.

For the thermodynamic approach, energy balance was considered. Built-in functions of EES for the heat capacity and molar mass was utilized in order to solve the heat of each gaseous

substance entering and leaving the system. For the solids, heat capacities, ratio between methane and calcium oxide, and the mass ratio between catalyst, dolomite (Mg-O) and calcium oxide were given.

For the heat transfer of the inlet and outlet substances, Eq. (25) was used. The reference system for the heat transfer was SATP.

### 3.4.1.2 Regenerator

The simulation of the regenerator was set to result in the heat need of the regenerator or *Heat Provided* as shown in Figure 14. Thus, the temperature of the different inlets and outlets must be set beforehand. When simulating the regenerator two reactions (calcination and reverse WGS) has to be taken into account. The substances in the regenerator are considered to reach the outlet temperature before reacting via calcination and reverse WGS. The ICE table for the regenerator is shown in Table 3. By implementing the ICE-table for the regenerator on Eq. (4), the equilibrium equations for calcination and reverse WGS were as follow:

$$K_{P,calcination} = (n_{CO_2,initial} + x_1 - x_2) \cdot \frac{P_{tot}}{(n_{H_2O,initial} + n_{H_2,initial} + x_1)} \quad (34)$$

$$K_{P,reverse\ WGS} = \frac{(x_2)(n_{H_2O,initial} + x_2)}{(n_{CO_2,initial} + x_1 - x_2)(n_{H_2,initial} - x_2)} \quad (35)$$

For the calcination, solid-state substances do not apply a partial pressure and is therefore not included in Eq. (34) and Eq. (35)

Table 3. ICE-table for reactions taking place in the regenerator. Where  $x_1$  and  $x_2$  represent the change in steam methane reformation (Eq. (4)) and (Eq. (4)) reverse water gas shift (Eq. (2)) respectively

<i>Substances</i>	<i>Initial (mol)</i>	<i>Change (mol)</i>	<i>Equilibrium (mol)</i>
$H_2$	$n_{H_2,initial}$	$-x_2$	$n_{H_2,initial} - x_2$
$H_2O$	$n_{H_2O,initial}$	$x_2$	$n_{H_2O,initial} + x_2$
$CO_2$	0	$x_1 - x_2$	$n_{CO_2,initial} + x_1 - x_2$
$CO$	0	$x_2$	$x_2$
$CaO$	$n_{CaO,initial}$	$x_1$	$n_{CaO,initial} - x_3$
$CaCO_3$	$n_{CaCO_3,initial}$	$-x_1$	$n_{CaCO_3,initial} + x_3$
Total	$n_{H_2O,initial} + n_{H_2,initial}$	$x_1$	$n_{H_2O,initial} + n_{H_2,initial} + x_1$

The amount of water and hydrogen entering the regenerator is decided by the outlet gas composition (%mol) wanted by the user. Since solids from the reformer are thought to be transported to the regenerator, the composition of the solids must be considered. The calcined dolomite is at this stage partially carbonated dolomite.

As previously stated, the regenerator simulation was set to result in the heat need of the total system. The heat need is generated from a simplified catalytic burner in the simulation. This has no direct interaction with the substances in the regenerator. Since the temperatures of the regenerators are fixed the heat need will be the only independent variable in the energy balance.

### 3.4.4 SOFC

In an ideal situation, a SOFC with high temperature (1000°C) is preferred in the ZEG-technology due to high quality waste heat for regenerating sorbent [3]. However, due to risk and complexity issues the current SOFC configuration used in ZEG plants run at a lower temperature (830°C). With a SOFC running at a lower temperature, a catalytic burner is needed to increase the temperature of the cathodic airflow [3].

An illustration of the control surface for the SOFC is shown in Figure 15. The SOFC has two inlets for gas, one for the cathode and one for the anode. The inlet of the anode is the reformat gas. The reformat gas is set as the gas coming out of the reformer in the simulation. Since the cathode requires oxygen, air with a composition (mole basis) of 80% nitrogen and 20% oxygen is thought to be entering the cathode. The cathodic flow is a value that depends on the oxygen utilization (OU) as shown in Eq. (13). The air exiting the cathode is set to enter the catalytic burner as shown in Figure 12.

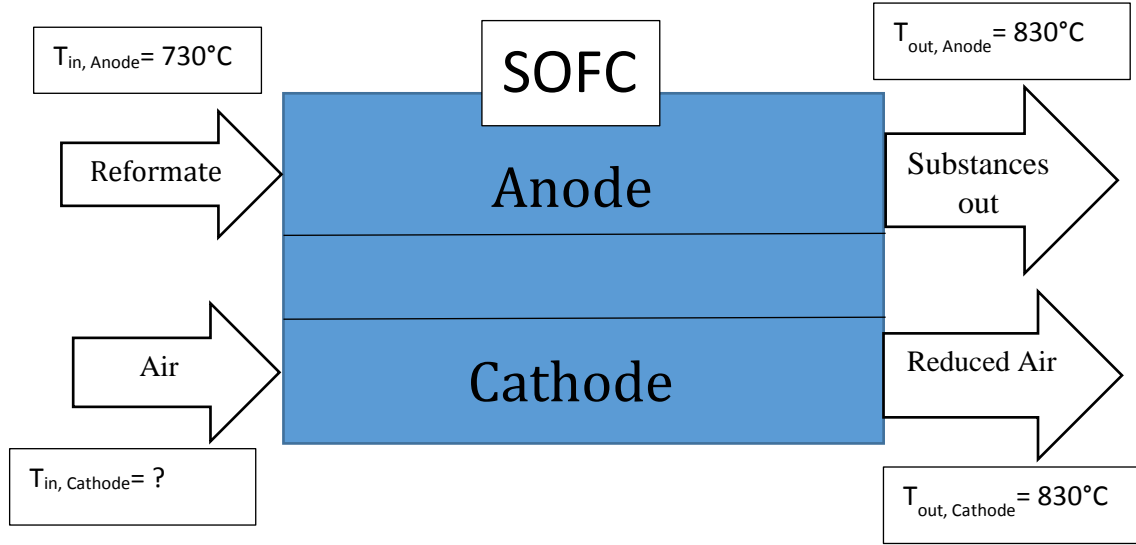


Figure 15. Control surface for the SOFC

For the reformat (outlet gas of reformer) entering the SOFC further SMR and WGS was applied through equilibrium. Since the temperature for the SOFC is higher than the reformer (830°C) and the carbon dioxide is captured in the reformer, equilibrium was applied. The ICE-table for the equilibrium is shown in Table 4. The data from Table 4 is applied to Eq. (20) and the equilibrium equation for SMR and WGS and we get the following equations:

$$K_{P,SR} = \frac{(x_1 - x_2)(n_{H_2,initial} + 3x_1 + x_2)^3}{(n_{CH_4,initial} - x_1)(n_{H_2O,initial} - x_1 - x_2)} \cdot \frac{P_{tot}^2}{(n_{H_2O,initial} + n_{H_2,initial} + n_{CH_4,initial} + n_{CO_2,initial} + 2x_1)^2} \quad (36)$$

$$K_{P,WGS} = \frac{(n_{CO_2,initial} + x_2)(n_{H_2,initial} + 3x_1 + x_2)}{(x_1 - x_2)(n_{H_2O,initial} - x_1 - x_2)} \quad (37)$$

Table 4. ICE table for the SOFC where  $x_1$  and  $x_2$  represent the change in steam methane reformation and (Eq. (1)) water gas shift (Eq. (2)) respectively

<b>Substances</b>	<b>Initial (mol)</b>	<b>Change (mol)</b>	<b>Equilibrium (mol)</b>
$H_2$	$n_{H_2,initial}$	$3x_1 + x_2$	$n_{H_2,initial} + 3x_1 + x_2$
$H_2O$	$n_{H_2O,initial}$	$-x_1 - x_2$	$n_{H_2O,initial} - x_1 - x_2$
$CH_4$	$n_{CH_4,initial}$	$-x_1$	$n_{CH_4,initial} - x_1$
$CO_2$	$n_{CO_2,initial}$	$x_2$	$n_{CO_2,initial} + x_2 - x_3$
$CO$	$n_{CO,initial}$	$x_1 - x_2$	$n_{CO,initial} + x_1 - x_2$
Total	$n_{H_2O,initial} + n_{CH_4,initial}$ $+ n_{CO_2,initial}$ $+ n_{H_2,initial}$	$2x_1$	$n_{H_2O,initial} + n_{CH_4,initial}$ $+ n_{CO_2,initial}$ $+ n_{H_2,initial} + 2x_1$

The cell voltage was calculated through Eq. (11). The SOFC manufacturer for ZEG Power provided the characteristics of the voltage and current. Assuming only ohmic losses through the electrolyte Eq. (11) can be written as:

$$V = V_{Nernst} - \eta_{ohm} \quad (38)$$

The ohmic losses through a cell is defined as [11]:

$$\eta_{ohm} = i \cdot r \quad [V] \quad (39)$$

where  $i$  is the current density and  $r$  is the area specific resistance.

The generation of electric power is calculated by Eq. (15). Since the current for one cell is calculated through Eq. (14) the assumption made is that the total molar flow is over one cell. With the current over one cell and cell voltage set to be constant, stack configuration is not necessary. This assumed scenario makes it easier to calculate the power generated for any fuel input.

The heat loss of the SOFC was set as a fraction of the power generated:

$$\dot{Q}_{loss} = (P_{el}) * loss \quad 0 \leq loss \leq 1 \quad (40)$$

### 3.4.5 Catalytic burner

The cathodic flow exiting the SOFC is thought to be entering the regenerator through a heat exchanger. Since the regeneration of sorbents requires a temperature of 850°C and cathodic flow of the SOFC can reach a maximum temperature of 830°C, a catalytic burner is implemented. The catalytic burner performs a combustion of methane with surplus air. In this, the mass flow of air is much bigger than the methane flow. Therefore, we consider complete combustion of methane, as shown in the following equation:



The setup of the catalytic burner is shown in Figure 16. By Figure 16, we can see that all the temperatures is set so that the energy balance of the system dictates the mass of the different substances by Eq. (25) and Eq. (26).

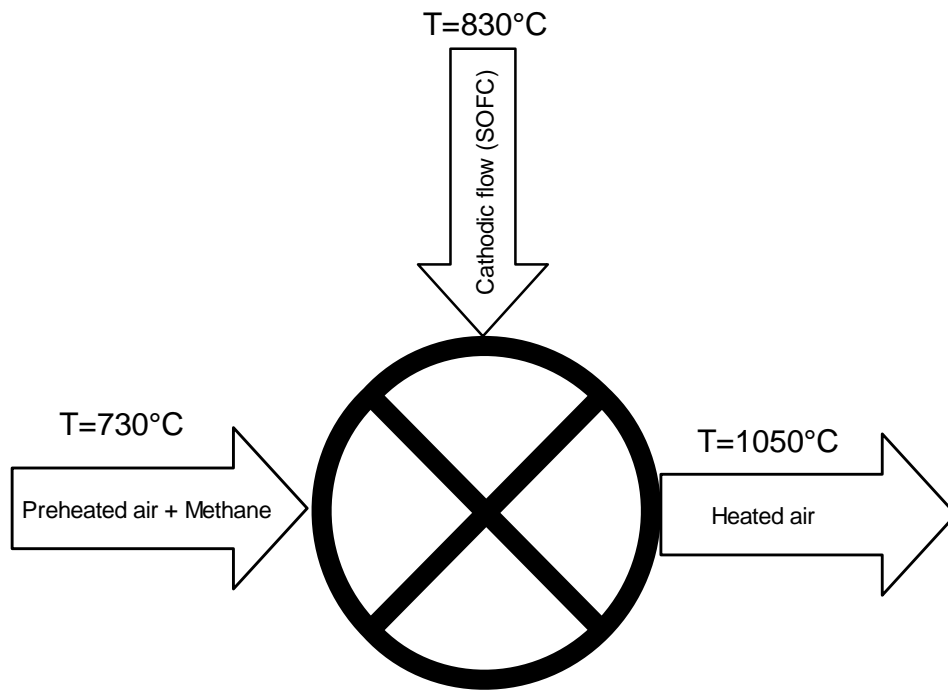
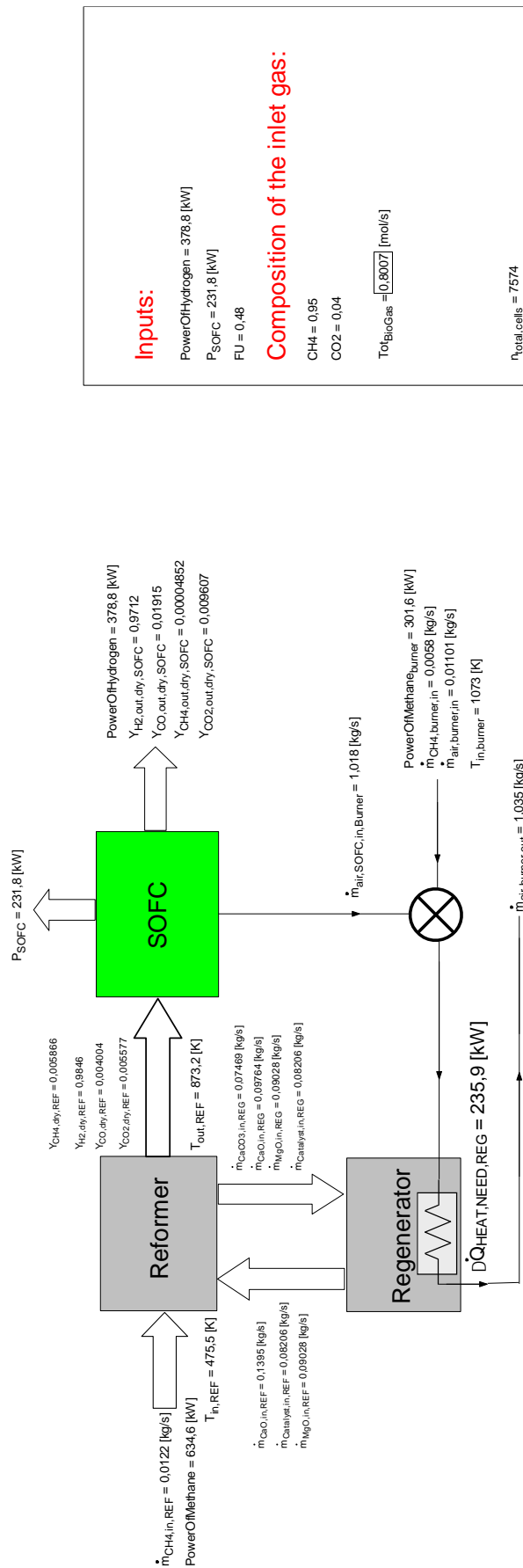


Figure 16. A schematic of the model setup for the catalytic burner in EES

## 4. Simulation performance

A validation of the model is carried out, where the most significant values of the simulation were compared to earlier studies. Once validated the model, the flexibility of the simulation tool for different operating conditions is furtherly tested through sensitivity analyses showing the capacity of the ZEG-technology.

The diagram made for the simulation is shown in Figure 17. This diagram is made to illustrate the process. The intension was also to create a user-friendly interface so that different users may generate and gather data as they please. The user-friendly interface contains a scheme of the process, the main results as well as access to input values. The full list of equations for the model can be viewed in Appendix B.



**Inputs:**  
 PowerOfHydrogen = 378,8 [kW]  
 P<sub>SOFC</sub> = 231,8 [kW]  
 FU = 0,48

**Composition of the inlet gas:**  
 CH<sub>4</sub> = 0,95  
 CO<sub>2</sub> = 0,04

To<sub>BioGas</sub> = 0,8007 [mol/s]

η<sub>total, cells</sub> = 7574

h<sub>CoGeneration</sub> = 0,65

h<sub>StandAlone</sub> = 0,76

Figure 17. Program made in EES for illustration of model and interactive simulation of the ZEG Power technology. This diagram show the output of the simulation on the ZEG400 configuration.

## 4.1 Model validation

The most significant values the ZEG-technology simulations were compared with the results from the ZEG400-project and the BioZEG-project. For both these cases, the composition of the inlet gas was:

- 95% CH<sub>4</sub>
- 5% CO<sub>2</sub>

For the SOFC, the FU, OU and heat loss was set accordingly to the previous simulation. In addition, the molar flow of the biogas being fed to the regenerator was set to the value given in the previous simulation. The heat loss for the SER was considered non-existent, as it was for the previous simulations. The amount of mass circulating in the system was set as a ratio between the calcium oxide and the methane, and was set to be equal for both cases. The full list of solutions generated in EES for the ZEG400 and BioZEG can be viewed in Appendix C and D.

For comparison of both simulations results deviating with less than 3% was considered as a good result. This choice is based on the complexity of previous simulations.

The results of the simulation is shown in Table 5 in comparison with IFE's data. As seen from Table 5, the data for the SOFC is not included. This decision was made based on that the SOFC was not connected to the SER for the BioZEG plant.

Table 5. ZEG power 50 kW plant data for comparison of EES model

	<b>EES Model</b>	<b>Previous Model</b>		<b>Deviation (%)</b>
<b>REFORMER</b>	<b>Value</b>	<b>Value</b>	<b>Unit</b>	
Temperature in	202	200	[°C]	1,0
Total molar flow reformatate	0,243	0,242	[mol/s]	0,49
H <sub>2</sub> -flow out	0,158	0,159	[mol/s]	0,88
H <sub>2</sub> -yield	3,89	3,89	mole H <sub>2</sub> /mole CH <sub>4</sub>	0
Power of hydrogen	38,2	38,5	[kW]	0,78
Solid mass flow out	0,019	0,021	[kg/s]	9,5
<b>REGENERATOR</b>				
Steam flow in	0,123	0,133	[mol/s]	7,4
H <sub>2</sub> -flow in	0,0028	0,0027	[mol/s]	3,7
CO <sub>2</sub> -flow out	0,0386	0,0363	[mol/s]	6,4
Heat need (Heat Exchanger)	12,8	12,2	[kW]	4,9

Table 5 shows that most of the values are well within range of the margin of error chosen (3%). The values of *Steam flow in*, *H<sub>2</sub>-flow in*, *CO<sub>2</sub>-flow out* and *Heat need (Heat Exchanger)* for the regenerator are deviating above the margin of error chosen. The inlet gas flow in the regenerator relies upon the composition of the outlet gas, and data provided did not contain information on the outlet gas composition of the regenerator. Therefore, guessing the outlet composition was implemented in order to attain an approximation of the outlet flow of the different gases in the regenerator. This is not an accurate method in attaining results for the simulation. With this said, the deviations are not immense when considering the complexity of previous simulations.



The value of *Solid mass flow out* is controlled by a ratio between calcium oxide and methane. Though this value differs for both the ZEG400 and BioZEG, the decision to hold it constant for both cases is based on information given for the previous simulations saying that the latest models are more optimized. Also, the changing of the ratio between calcium oxide and methane is not logical for the model made in EES since the model does not consider fluid dynamics and should work for different configurations of the ZEG-technology.

Table 6 shows the comparing of ZEG400 model against the simulation done in EES. The input variables of the simulation in EES were set to match the data given in previous models.

Table 6. ZEG Power 400 kW plant data for comparison of EES model

	<b>EES Model</b>	<b>Previous Model</b>		<b>Deviation (%)</b>
<b>REFORMER</b>	<b>Value</b>	<b>Value</b>	<b>Unit</b>	
Temperature in	201	200	[°C]	0,50
Total molar flow out	4,58	4,58	[mol/s]	0
H <sub>2</sub> -flow out	2,96	2,91	[mol/s]	1,71
H <sub>2</sub> -yield	3,89	3,82	mole H <sub>2</sub> /mole CH <sub>4</sub>	1,83
Power of hydrogen	716	703	[kW]	1,84
Solid mass flow out	0,3484	0,3372	[kg/s]	3,32
<b>REGENERATOR</b>				
Steam flow in	1,04	1,02	[mol/s]	1,96
H <sub>2</sub> -flow in	0,021	0,021	[mol/s]	0
CO <sub>2</sub> -flow out	0,729	0,724	[mol/s]	0,69
Heat need (Heat Exchanger)	236	236	[kW]	0
<b>SOFC</b>				
Fuel utilization	48	48	[%]	0
Oxygen utilization	10,2	10,2	[%]	0
Fuel power	728	728	[kW]	0,06
Power SOFC module	231,8	230	[kW]	0,78
Heat SOFC Module	117,9	116	[kW]	1,63
Exhaust fuel power	378	382	[kW]	1,05
Cathode inlet temperature	751	752	[°C]	0,13

As one may see, most values generated by the simulation in EES are matching the previous models within the range. That is, within a 3% margin of error. The value of *Solid mass flow out* for the reformer shows a 3,3% deviation from the previous models. This result is solely dependent on the amount of CO<sub>2</sub> converted to calcium carbonate in the carbonation reaction (reaction (3)) since the amount of solid mass going into the reformer is pre-set in the EES simulation. The amount of CO<sub>2</sub> converted to calcium carbonate for the previous simulations takes into account the evolution of the reaction. When having stated this, the deviation is not considerable with respect to the complexity of the previous simulation compared to the simulation made in EES. The results in general show good reliability for the simulation made in EES.

## 4.1 Sensitivity analysis

Sensitivity analysis is carried out in order to assess the operational capacity of the ZEG-technology. For instance, checking of a dependent variable upon changing the independent variable of a function, demonstrates the behaviour of the function. The sensitivity analysis for the EES model was done in order to see if the simulation behaves according to ZEG-technology in different scenarios.

For the sensitivity analysis the following scenarios was tested:

- The inlet temperature of reformer vs. the CO<sub>2</sub> content in the fed biogas
- The heat need in the regenerator and standalone efficiency vs. the heat loss in the regenerator
- The co-generation efficiency vs. the fuel utilization of the SOFC
- The co-generation efficiency vs. the oxygen utilization
- The inlet temperature of the catalytic burner vs. standalone efficiency
- The efficiency of a standalone plant the inlet temperature of catalytic burner
- The co-generation efficiency of the plant and the mass flow of methane into the catalytic burner vs. the outlet temperature of the SOFC

All plots shown in Figure 18, 19, 20, 21, 22, 23 and 24 are generated from the parametric tables in Appendix A. For the standalone cases, FU was set to 0,1%, as this is the lowest pre-setting of the FU the EES model allows.

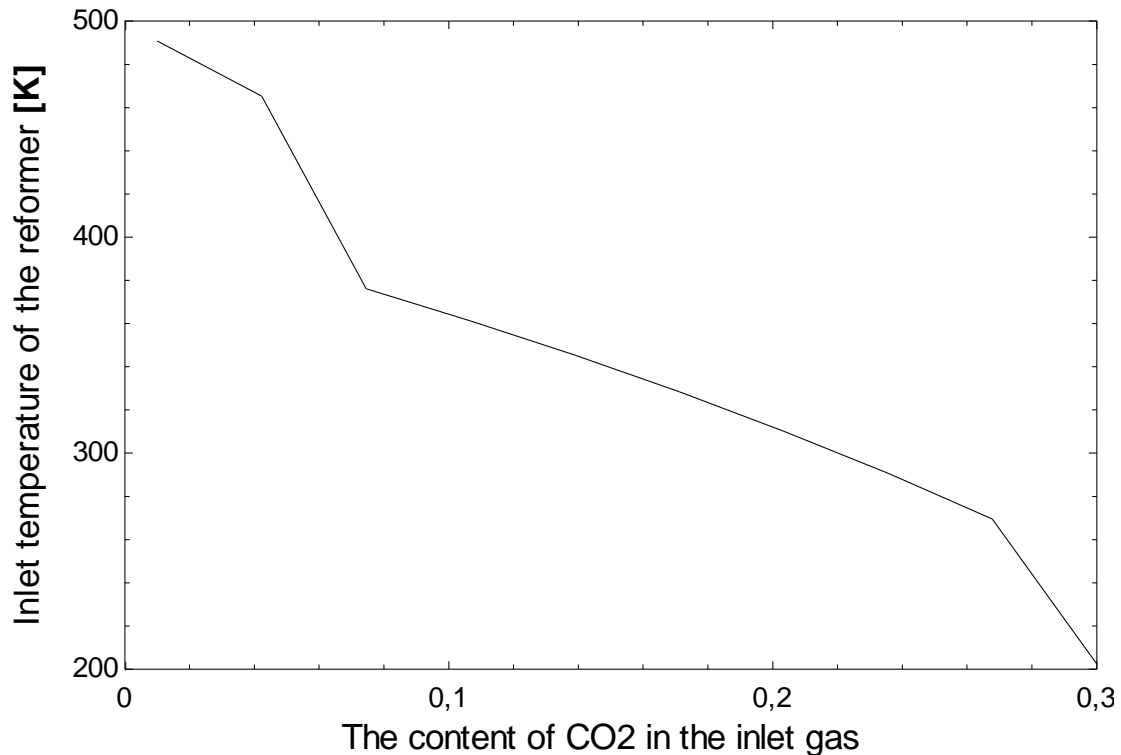


Figure 18. Plot of composition of CO<sub>2</sub> in biogas versus the inlet temperature of the reformer

Figure 18 gives us a perspective of the EES simulation reaction upon increasing the CO<sub>2</sub> content in the biogas. This is highly relevant since raw biogas usually contains up to 40% CO<sub>2</sub>. The biogas that is fed to the regenerator is refined biogas (>90% CH<sub>4</sub>), meaning that most of the CO<sub>2</sub> in the raw biogas is removed. As Figure 18 displays, the temperature decreases when increasing the CO<sub>2</sub> content of the biogas. This is a consequence of the decreasing of reaction (1) and increasing of reaction (3). The heat of formation for the reformer becomes more exothermic and since the inlet temperature of the reformer is set to be a dependent variable, the inlet temperature of the reformer decreases accordingly to Eq. (25). This is not a realistic scenario, since the inlet temperature is always presumed to be 200°C. When feeding the reformer using biogas with high CO<sub>2</sub> content, it is more sensible to remove heat from the regenerator in order to sustain the inlet temperature to 200°C.

One may see that the curve of Figure 18 is not completely linear but has linear regions. This is related to the phase change of water at the inlet of the reformer.

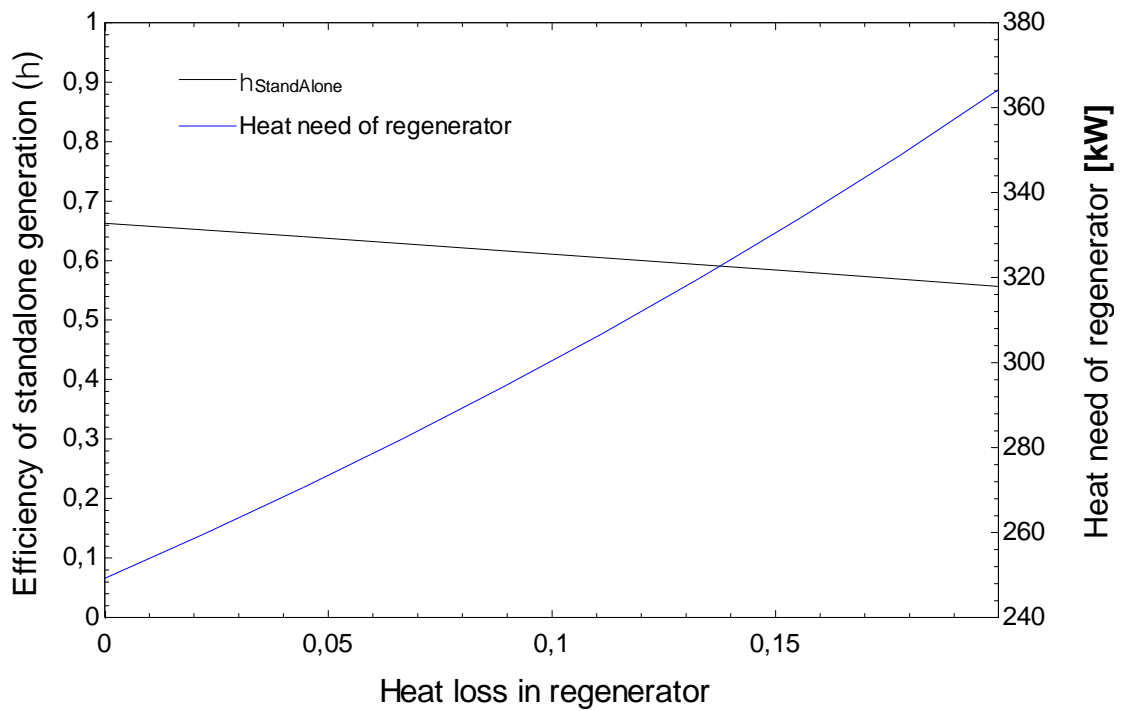


Figure 19. Plot of the heat loss in the regenerator against the heat need of the regenerator and the standalone efficiency of the SER

Figure 19 shows the heat need of the regenerator and the efficiency of standalone hydrogen production as a function of heat loss in the regenerator. When increasing the heat loss in the regenerator, the heat need of the regenerator is expected to increase by energy balance (Eq. (25)). Since the heat need increases for the regenerator, the catalytic burner has to increase the heat transfer to the regenerator, and thereby increasing the amount of methane used in the catalytic burner. This decreases the efficiency, which is govern by the amount of methane being utilized in the ZEG-technology, by Eq. (28).

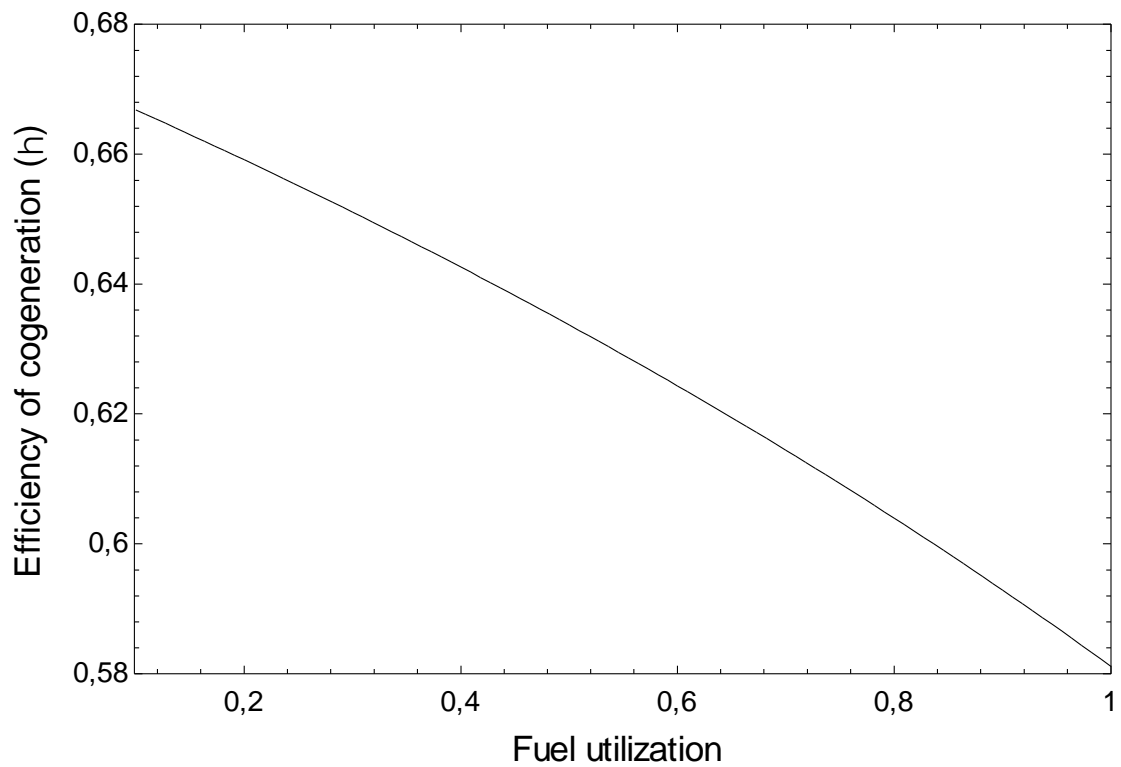


Figure 20. Plot of the fuel utilization of the SOFC against the efficiency of co-generation

Figure 20 shows the efficiency of co-generation as a function of fuel utilization. The fuel utilization decides the power generation of the SOFC. When increasing the fuel utilization of the SOFC to 100%, that is, when all exiting fuel from the SER is consumed by the SOFC, the efficiency of co-generation is to follow Eq. (29). Since the power generation does not utilize the full potential lower heating value of the fuel, the efficiency of co-generation will decrease. When the fuel utilization goes towards zero the plant will be in standalone generation of hydrogen and the co-generation efficiency will approach the standalone efficiency.

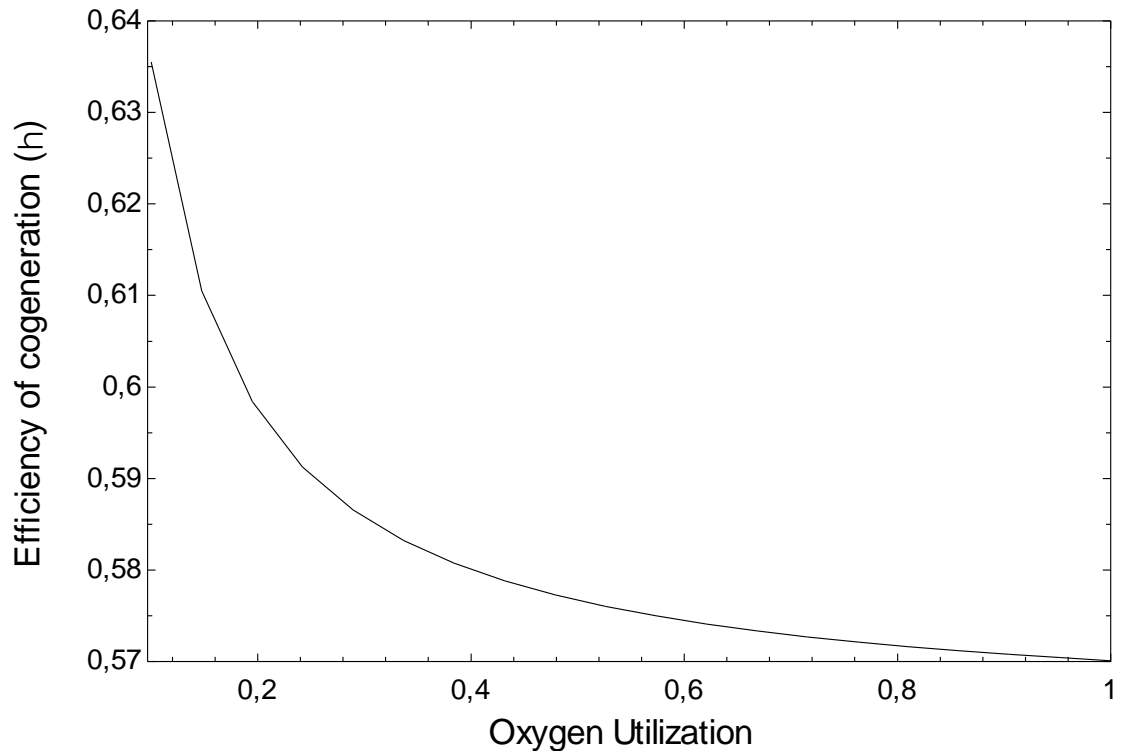


Figure 21. Plot of the co-generation efficiency with varying oxygen utilization

Figure 21 shows the co-generation efficiency as a function of oxygen utilization. The oxygen utilization decides the airflow into the SOFC, by Eq. (13). Hence, the cathodic outlet gas flow of the SOFC is also decided by the oxygen utilization. Since the cathodic outlet gas flow is set to contribute to the catalytic burner with heated air, and thereby effects the methane consumption of the catalytic burner, the efficiency of co-generation is influenced by the oxygen utilization.

Though it may seem, from Figure 21, that having a low oxygen utilization is desirable in a ZEG-technology configuration, the risk of high mechanical stresses and pressure losses at the cathode of the SOFC is high when the cathodic flow increases.

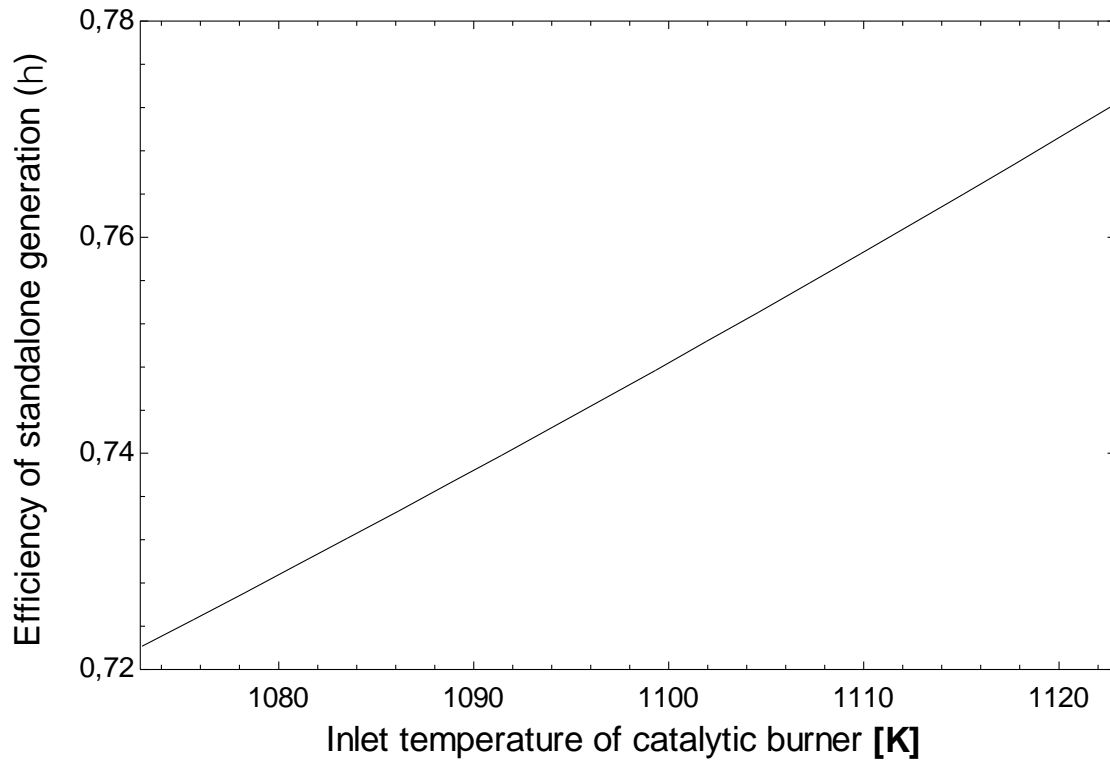


Figure 22. Plot of the efficiency of standalone generation versus the temperature at the inlet of the catalytic burner

Figure 22 shows the function of standalone efficiency upon varying the inlet temperature of the catalytic burner. Changing the temperature of the preheated air, effects the amount of methane needed to increase the temperature of the air for further use in the regeneration of sorbents. The amount of methane governs the efficiency of standalone operation by Eq. (28). This shows the case of when all of the air is being supplied by the SOFC.

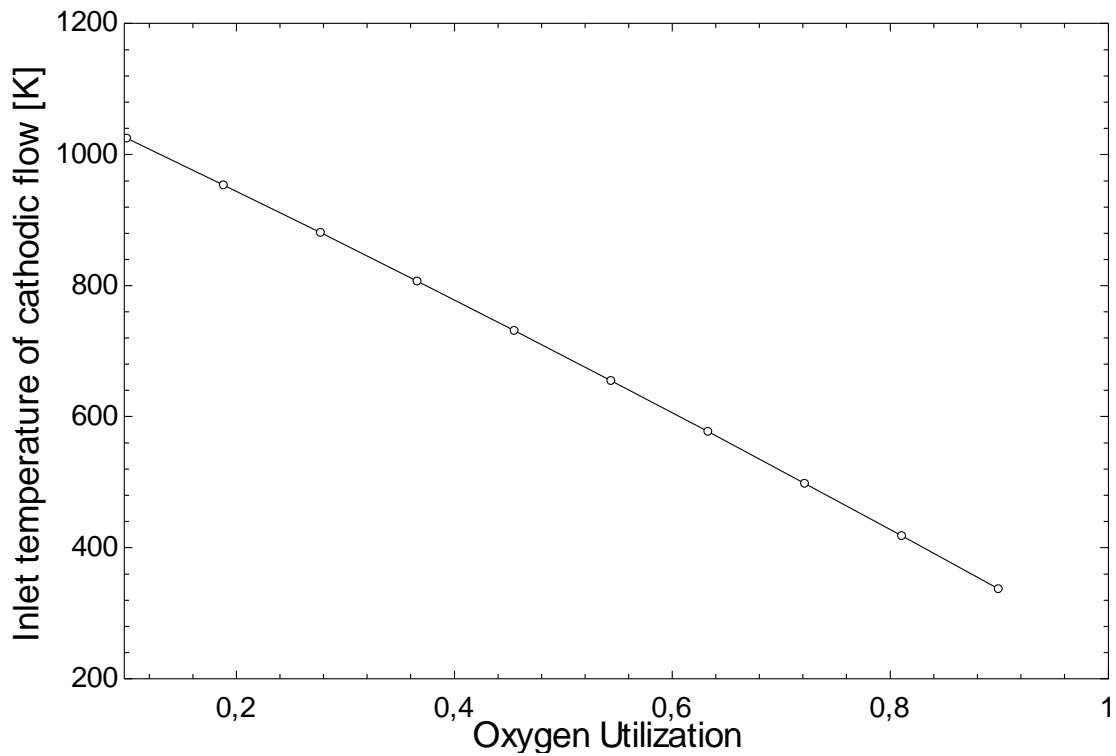


Figure 23. Plot of the effect of oxygen utilization on the cathodic inlet temperature

Figure 23 shows the inlet temperature of the cathodic flow as a function of oxygen utilization. This relation should follow the relation of Eq. (23). Since the cathodic airflow is decreasing through Eq. (13) and the heat transfer is constant through the energy balance, one can expect that the inlet temperature is decreasing. The incoming air at the cathode of the SOFC is thought to be heated up by waste heat from the heat exchanger immersed in the regenerator, but when the two systems are not connected the system will require additional heating of the air going into the SOFC.



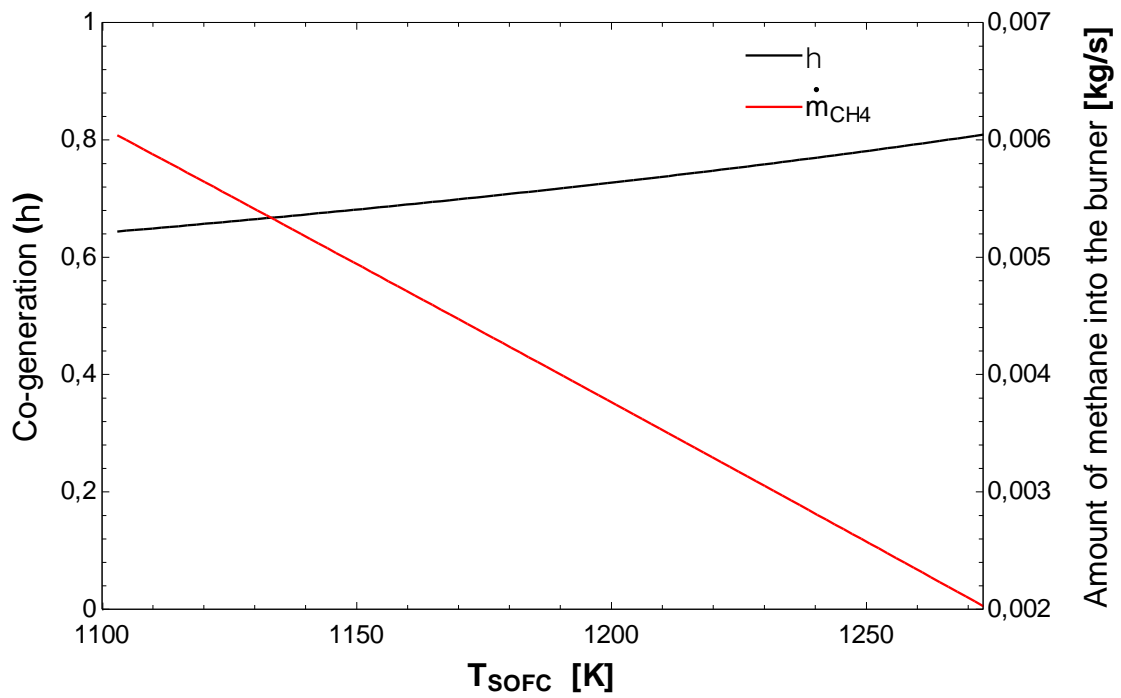


Figure 24. The influence of the SOFC temperature on the co-generation efficiency and methane used in the catalytic burner

In Figure 24, the temperature of the SOFC is plotted against the total efficiency of the plant and the mass flow of methane into the catalytic burner. The rising of the temperature causes the catalytic burner to lower its consumption of methane by energy balance and hence the efficiency of the whole plant rises by Eq. (25). To have an SOFC operating at 1000°C was, as mentioned, the initial plan of ZEG Power. With Figure 24, it can be shown that if the technology allows a SOFC operating at 1000°C, the simulation done in EES will allow it.

## 5. Conclusion

This thesis was made over a course of 4 months. The main idea was to optimize a previously done simulation done on the SER to a more complete simulation of EES, including the SOFC and the catalytic burner. Therefore, a similar model was made in EES, taking into account the different technologies that ZEG Power utilizes. The mission of constructing a zero-dimensional model was accomplished within the given time frame. This type of models requires assumptions about the pressures and volumes of the system. Decisions were made towards what approximations one may consider in order to make a good model for the ZEG-technology.

The possibility of using a more accurate method of calculating the heat of each substance is present in EES. However, the decision of using the method of *average heat capacity* was made in order to save time and gives a good approximation of the transferred heat. The limited timeframe did not allow expanding the program and including some of the essential things for the BOP. The BOP for the model made is very simplified when in reality the ZEG-technology includes a more complex scheme in which several heat exchangers and compressors for the gas has to be included.

The sensitivity analysis for the model made in EES show that the simulation performs according to ZEG-technology. Dependent variables do not act in an unexpected way upon changing independent variables. This shows that the simulation upholds good capacity.

The simulation of the two cases gave relative good results in comparison with previous models. For a zero-dimensional model, one may expect to have some bigger deviations for some outputs than the results show. The results of the simulation show that the biggest deviation of the most significant values was around 9,5% for the BioZEG compared to previous models. This is not a noteworthy deviation when one takes into account the complexity of the previous models compared to the model created in EES. Whilst for the ZEG400 the biggest deviation was 3,3% which shows that the model holds good quality when compared to the latest version of the ZEG-technology simulations. The simulation was made as a tool for preliminary research of the ZEG-technology in different configurations and that has been accomplished. Therefore, it can be concluded that the thesis goal was accomplished and the produced model is complete and holds good quality.



## 6. Further work

The program made in EES was prepared as a tool for analyzing the different aspects of the ZEG-technology. The main purpose of the simulation was to analyze how the technology reacts when altering certain parameters and have a convenient tool for early stage studies as support for research proposals and patenting. Therefore, there is no intention of generating a tool, which will replace more accurate simulations done in EES, MATLAB and HYSYS. However, the model can certainly be optimized. For example, other part of the High Temperature System (e.g. heat exchangers) and of the Balance of Plant (e.g. air compressor) could be included to have a more accurate sensitivity analysis of the need for more precise simulation on the heat transfer system inside the regenerator can also be addressed. The configuration used so far includes a u-tube heat exchanger imbedded in the fluidized bed. Additional simulation including the relations between the heat transfer coefficients and the exchange (and thus the fuel used) could allow studying the effect of alternative configurations (e.g. use of pulse combustion technology) on the performance of the plants. Therefore, implementing additional thermodynamic equation for the heat exchange in the simulation would be desirable. The BoP for the BioZEG-project is shown in Figure 25.

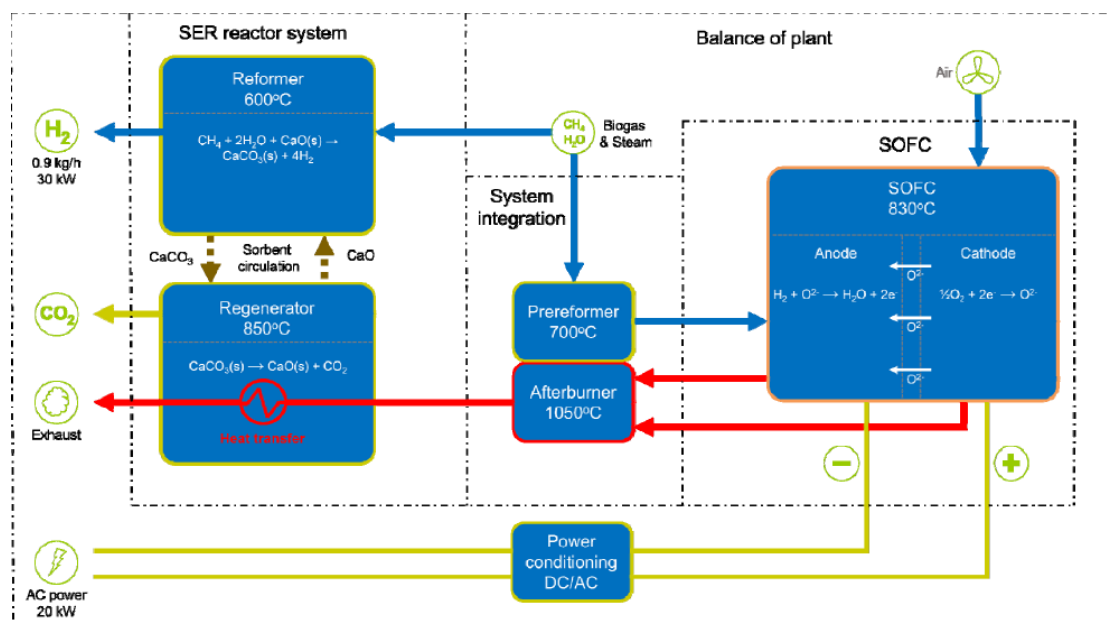


Figure 25. Simplified process flow diagram of the BioZEG plant including additional BOP [21].

The option of adding several dimensions to the simulation is also possible and EES allows one to include fluid dynamics. This would improve the precision of the simulation and simultaneously give the model another aspect.



## References

1. Field, C.B., V.R. Barros, D.J. Dokken, K.J. Mach, M.D. Mastrandrea, T.E. Bilir, M. Chatterjee, K.L. Ebi, Y.O. Estrada, R.C. Genova, B. Girma, E.S. Kissel, A.N. Levy, S. MacCracken, P.R. Mastrandrea, and L.L.White (eds.), *Climate Change 2014: Impacts, Adaptation, and Vulnerability; Part A: Global and Sectoral Aspects*, V.R.B. Christopher B. Field, Editor. 2014, Intergovernmental Panel on Climate Change.
2. Metz, B., et al., *Carbon dioxide capture and storage*. 2005.
3. Andresen, B., et al., *BioZEG – Pilot Plant Demonstration of High Efficiency Carbon Negative Energy Production*. Energy Procedia, 2014. **63**: p. 279-285.
4. Øystein Ulleberg, Julien Meyer, Jon Eriksen, Arnstein Norheim, Jan C. Gjerløw, *Hynor Lillestrøm – A Renewable Hydrogen Station & Technology Test Center*. WHEC 2014, 2014.
5. Meyer, J., et al., *Techno-economical study of the Zero Emission Gas power concept*. Energy Procedia, 2011. **4**: p. 1949-1956.
6. Johnsen, K., *Sorption-Enhanced Steam Methane Reforming in Fluidized Bed Reactors*, in *Materials Science and Engineering*. 2006, Norwegian University of Science and Technology: Norwegian University of Science and Technology. p. 172.
7. Andresen, B., *ZEG Power - an energy technology revolution*, in *Cleantuesday*. 2012, ZEG Power: Oslo.
8. Johnsen, K., et al., *Sorption-enhanced steam reforming of methane in a fluidized bed reactor with dolomite as -acceptor*. Chemical Engineering Science, 2006. **61**(4): p. 1195-1202.
9. Bottino, A., et al., *Steam reforming of methane in equilibrium membrane reactors for integration in power cycles*. Catalysis Today, 2006. **118**(1–2): p. 214-222.
10. Kevin Huang, J.B.G., *Solid oxide fuel cell technology: Principles, performance and operations*. 2009: Woodhead Publishing Limited.
11. Chris Rayment, S.S., *Introduction to Fuel Cell Technology*. 2003, Department of Aerospace and Mechanical Engineering: Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, IN 46556, U.S.A.
12. Nicola Di Giulio, J.S., Øystein Ulleberg, Bjørg Andresen. Julien Meyer,, *High efficiency carbon negative energy production - BioZEG power plant operation*, in *Trondheim Conference on CO2 Capture, Transport and Storage*. 2015, ZEG Power: Trondheim, Norway.
13. Cambridge, U.o. *Fuel Cells*. 2015; Available from: <http://www.doitpoms.ac.uk/tlplib/fuel-cells/printall.php>.
14. Richard E. Sonntag, C.B., *Introduction to engineering thermodynamics*. Second ed. 2007.
15. Yang, S., et al., *Electrochemical Analysis of an Anode-Supported SOFC*. International Journal of ELECTROCHEMICAL SCIENCE, 2013. **8**.
16. Winter, M. and R.J. Brodd, *What Are Batteries, Fuel Cells, and Supercapacitors?* Chemical Reviews, 2004. **104**(10): p. 4245-4270.
17. Raymond Chang, J.O., *General Chemistry: The essential concepts*. Sixth ed. 2011, New York: McGraw-Hill.
18. *Chemical Equilibrium*. 2016; Available from: <http://chemistry.tutorvista.com/physical-chemistry/chemical-equilibrium.html>.
19. E. John Finnemore, J.B.F., *FLUID MECHANICS WITH ENGINEERING APPLICATIONS*. 10 ed. 2002: McGraw-Hill Higher Education.
20. McAllister, S., J.Y. Chen, and A.C. Fernandez-Pello, *Fundamentals of Combustion Processes*. 2011: Springer New York.

21. Paul Charbonneau, B.K., *EES: Engineering equation solver for Microsoft Windows operating systems*. 2002: Fchart.

## Appendix A

Parametric tables for the plots made in EES. The plots were made based on the ZEG400 simulation.

1..20	1 LOSS <sub>REG</sub>	2 $\eta_{\text{StandAlone}}$	3 $\Delta Q_{\text{dot,HEAT,NEED}}$ [kW]
Run 1	0	0,66	249,2
Run 2	0,02105	0,65	259,1
Run 3	0,04211	0,64	269,4
Run 4	0,06316	0,63	280,2
Run 5	0,08421	0,62	291,5
Run 6	0,1053	0,61	303,4
Run 7	0,1263	0,60	315,8
Run 8	0,1474	0,59	328,8
Run 9	0,1684	0,57	342,5
Run 10	0,1895	0,56	356,9
Run 11	0,2105	0,55	372
Run 12	0,2316	0,54	388
Run 13	0,2526	0,53	404,9
Run 14	0,2737	0,51	422,7
Run 15	0,2947	0,50	441,7
Run 16	0,3158	0,49	461,8
Run 17	0,3368	0,48	483,1
Run 18	0,3579	0,46	505,9
Run 19	0,3789	0,45	530,2
<b>Run 20</b>	<b>0,4</b>	<b>0,44</b>	<b>556,2</b>

1..10	1 CO <sub>2</sub>	2 $T_{\text{in,REF}}$ [K]
Run 1	0,01	490,8
Run 2	0,04222	465,2
Run 3	0,07444	376
Run 4	0,1067	361,2
Run 5	0,1389	345,3
Run 6	0,1711	328,4
Run 7	0,2033	310,2
Run 8	0,2356	290,6
Run 9	0,2678	269,5
<b>Run 10</b>	<b>0,3</b>	<b>202,3</b>

Figure 26. Parametric tables for Figure 16 and 17



1..20	1 $\eta_{CoGeneration}$	2 OU
Run 1	0,64	0,1
Run 2	0,64	0,1474
Run 3	0,63	0,1947
Run 4	0,63	0,2421
Run 5	0,63	0,2895
Run 6	0,63	0,3368
Run 7	0,63	0,3842
Run 8	0,63	0,4316
Run 9	0,63	0,4789
Run 10	0,62	0,5263
Run 11	0,62	0,5737
Run 12	0,62	0,6211
Run 13	0,62	0,6684
Run 14	0,62	0,7158
Run 15	0,62	0,7632
Run 16	0,62	0,8105
Run 17	0,62	0,8579
Run 18	0,62	0,9053
Run 19	0,62	0,9526
Run 20	0,62	1

1..10	1 FU	2 $\eta_{CoGeneration}$
Run 1	0,1	0,72
Run 2	0,2	0,70
Run 3	0,3	0,68
Run 4	0,4	0,66
Run 5	0,5	0,64
Run 6	0,6	0,62
Run 7	0,7	0,60
Run 8	0,8	0,58
Run 9	0,9	0,55
Run 10	1	0,53

Figure 27. Parametric tables for Figure 18 and 19

1..10	1 $T_{in;burner}$ [K]	2 $\eta_{StandAlone}$	1..10	1 OU	2 $T_{in;cat;SOFC}$ [K]
Run 1	1073	0,73	Run 1	0,1	1024
Run 2	1079	0,73	Run 2	0,2	943,7
Run 3	1084	0,74	Run 3	0,3	861,7
Run 4	1090	0,74	Run 4	0,4	778,1
Run 5	1095	0,75	Run 5	0,5	692,8
Run 6	1101	0,75	Run 6	0,6	605,8
Run 7	1106	0,76	Run 7	0,7	517,2
Run 8	1112	0,77	Run 8	0,8	427,3
Run 9	1117	0,77	Run 9	0,9	336,6
Run 10	1123	0,78	Run 10	1	245,4

Figure 28. Parametric tables for Figure 20 and 21

1..10	1 $T_{SOFC}$ [K]	2. $m_{CH_4;burner,in}$ [kg/s]	3 $\eta_{CoGeneration}$
<b>Run 1</b>	1103	0,006021	0,64
Run 2	1122	0,005588	0,66
Run 3	1140	0,005153	0,67
Run 4	1159	0,004717	0,69
Run 5	1177	0,00428	0,71
Run 6	1196	0,003841	0,72
Run 7	1214	0,0034	0,74
Run 8	1233	0,002959	0,76
Run 9	1251	0,002516	0,78
Run 10	1270	0,002071	0,81

Figure 29. Parametric tables for Figure 22



# Appendix B

**Equations** made in EES for the simulation of the ZEG-technology.

## Model description:

**For this model there are some nomenclatures that needs explanation. REF is reformer. REG is regenerator. SOFC is solid oxide fuel cell.**

**The model contains data from previous simulations done by institute of energy technology, christian michelsen research prototech and anstalt für verbrennungskraftmaschinen.**

**Also, data for the equilibrium constants are from previous simulation in EES of the SER.**

**Some equations are to long to fit in the PDF file created by EES, so they may seem peculiar. Rest assured, they are written correctly**

## Conditions for the SER

$$T_0 = \text{ConvertTemp}(C; K; 25) \quad (1)$$

$$T_{out;REF} = \text{ConvertTemp}(C; K; 600) \quad (2)$$

$$T_{calc} = \text{ConvertTemp}(C; K; 850) \quad (3)$$

$$P = 1 \text{ [atm]} \quad (4)$$

## Inlet gas

$$CH_4 = 0,95 \quad (5)$$

$$CO_2 = 0,03 \quad (6)$$

$$Tot_{BioGas} = 0,8007 \text{ [mol/s]} \quad (7)$$

$$Ratio_{CaO;CH_4} = 3,27 \quad (8)$$

$$SteamCarbonRatio = 4 \quad (9)$$

$$\dot{n}_{CH_4;in;REF} = CH_4 \cdot Tot_{BioGas} \quad (10)$$

$$\dot{n}_{H_2O;in;REF} = \dot{n}_{CH_4;in;REF} \cdot SteamCarbonRatio \quad (11)$$

$$\dot{n}_{CO_2;in;REF} = CO_2 \cdot Tot_{BioGas} \quad (12)$$

$$\dot{n}_{N_2;in;REF} = N_2 \cdot Tot_{BioGas} \quad (13)$$

$$\dot{n}_{CaO;in;REF} = Ratio_{CaO;CH_4} \cdot \dot{n}_{CH_4;in;REF} \quad (14)$$

$$\dot{n}_{tot;in;REF} = \dot{n}_{CH_4;in;REF} + \dot{n}_{H_2O;in;REF} + \dot{n}_{CO_2;in;REF} + \dot{n}_{N_2;in;REF} \quad (15)$$

## Moles of each substance at the equilibrium

$$\dot{n}_{CH_4;eq;REF} = \dot{n}_{CH_4;in;REF} - x_1 \quad (16)$$

$$\dot{n}_{H_2O;eq;REF} = \dot{n}_{H_2O;in;REF} - x_1 - x_2 \quad (17)$$

$$\dot{n}_{CO;eq;REF} = x_1 - x_2 \quad (18)$$

$$\dot{n}_{H_2;eq;REF} = 3 \cdot x_1 + x_2 \quad (19)$$

$$\dot{n}_{CO_2;eq;REF} = \dot{n}_{CO_2;in;REF} + x_2 - x_3 \quad (20)$$

$$\dot{n}_{CaO;eq;REF} = \dot{n}_{CaO;in;REF} - x_3 \quad (21)$$

$$\dot{n}_{CaCO_3;eq;REF} = x_3 \quad (22)$$

$$\dot{n}_{tot;eq;REF} = \dot{n}_{CH_4;eq;REF} + \dot{n}_{H_2O;eq;REF} + \dot{n}_{CO;eq;REF} + \dot{n}_{H_2;eq;REF} + \dot{n}_{CO_2;eq;REF} \quad (23)$$

#### Equilibrium constant for the steam reformation

$$K_{p;SR} = \exp \left( \left( -26830 \frac{[K]}{T_{out;REF}} \right) + 30, 11 \right) \cdot 1 \text{ [atm}^2] \quad (24)$$

$$K_{p;SR} = \frac{\dot{n}_{CO;eq;REF} \cdot (\dot{n}_{H_2;eq;REF}^3) \cdot P^2}{\dot{n}_{CH_4;eq;REF} \cdot \dot{n}_{H_2O;eq;REF} \cdot ((\dot{n}_{tot;eq;REF})^2)} \quad (25)$$

#### Equilibrium constant for the water gas shift

$$K_{p;WGS} = \left( \exp \left( \left( 4160 \frac{[K]}{T_{out;REF}} \right) - 3, 798 \right) \right) \quad (26)$$

$$K_{p;WGS} = \left( \frac{(\dot{n}_{CO_2;eq;REF}) \cdot (\dot{n}_{H_2;eq;REF})}{\dot{n}_{H_2O;eq;REF} \cdot \dot{n}_{CO;eq;REF}} \right) \quad (27)$$

#### Equilibrium constant for the carbonation

$$K_{p;CO_2} = 1 \frac{[1/kPa]}{101, 325 \cdot 10^{\left( \frac{-8308 [K]}{1} T_{out;REF} + 7, 079 \right)}} \quad (28)$$

$$K_{p;CO_2} = \left( \frac{\dot{n}_{tot;eq;REF}}{\dot{n}_{CO_2;eq;REF} \cdot P \cdot \left| 101, 325000 \frac{kPa}{atm} \right|} \right) \quad (29)$$

#### Fractions at equilibrium

$$\dot{n}_{tot;dry;REF} = \dot{n}_{CH_4;eq;REF} + \dot{n}_{CO;eq;REF} + \dot{n}_{H_2;eq;REF} + \dot{n}_{CO_2;eq;REF} \quad (30)$$

$$Y_{CO_2;dry;REF} = \dot{n}_{CO_2;eq;REF} / \dot{n}_{tot;dry;REF} \quad (31)$$

$$Y_{CH_4;dry;REF} = \dot{n}_{CH_4;eq;REF} / \dot{n}_{tot;dry;REF} \quad (32)$$

$$Y_{CO;dry;REF} = \dot{n}_{CO;eq;REF} / \dot{n}_{tot;dry;REF} \quad (33)$$

$$Y_{H_2;dry;REF} = \dot{n}_{H_2;eq;REF} / \dot{n}_{tot;dry;REF} \quad (34)$$

$$LHV_{CH_4} = 52 \text{ [MJ/kg]} \cdot \left| 1000, 00000 \frac{kJ/kg}{MJ/kg} \right| \quad (35)$$

$$LHV_{H_2} = 120 \text{ [MJ/kg]} \cdot \left| 1000, 00000 \frac{kJ/kg}{MJ/kg} \right| \quad (36)$$

$$LHV_{CO} = 10 \text{ [MJ/kg]} \cdot \left| 1000, 00000 \frac{kJ/kg}{MJ/kg} \right| \quad (37)$$

$$\dot{m}_{CH_4;in;REF} = MW(CH_4) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CH_4;in;REF} \quad (38)$$

$$\dot{m}_{H_2O;in;REF} = MW(H_2O) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{H_2O;in;REF} \quad (39)$$

$$\dot{m}_{CO_2;in;REF} = MW(CO_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CO_2;in;REF} \quad (40)$$

$$\dot{m}_{CaO;in;REF} = MW(CaO) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CaO;in;REF} \quad (41)$$

$$\dot{m}_{CH_4;out;REF} = MW(CH_4) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CH_4;eq;REF} \quad (42)$$

$$\dot{m}_{CO_2;out;REF} = MW(CO_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CO_2;eq;REF} \quad (43)$$

$$\dot{m}_{CO;out;REF} = MW(CO) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CO;eq;REF} \quad (44)$$

$$\dot{m}_{H_2O;out;REF} = MW(H_2O) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{H_2O;eq;REF} \quad (45)$$

$$\dot{m}_{H_2;out;REF} = MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{H_2;eq;REF} \quad (46)$$

$$\dot{m}_{CaO;out;REF} = MW(CaO) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CaO;eq;REF} \quad (47)$$

$$\dot{m}_{CaCO_3;out;REF} = \dot{n}_{CaCO_3;out;REF} \cdot \left( (MW(Ca) + MW(CO_2) + MW(O)) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (48)$$

$$m_{solids;out;REF} = \dot{m}_{CaCO_3;out;REF} + \dot{m}_{Catalyst;out;REF} + \dot{m}_{MgO;out;REF} + \dot{m}_{CaO;out;REF} \quad (49)$$

$$m_{solids;in;REF} = \dot{m}_{Catalyst;in;REF} + \dot{m}_{MgO;in;REF} + \dot{m}_{CaO;in;REF} \quad (50)$$

### The internal energy of the inlet substances

$$C_{p;CH_4;in;REF} = c_p \left( \text{Methane}; P = P_0; T = \left( \left( \left( \frac{T_{in;REF} + T_0}{2} \right) \right) \right) \right) \quad (51)$$

$$C_{p;H_2O;in;REF} = c_p \left( \text{Steam}; P = P_0; T = \left( \left( \frac{T_{in;REF} + T_0}{2} \right) \right) \right) \quad (52)$$

$$C_{p;CO_2;in;REF} = c_p \left( \text{CarbonDioxide}; P = P_0; T = \left( \frac{T_{in;REF} + T_0}{2} \right) \right) \quad (53)$$

$$\dot{Q}_{CH_4;in;REF} = \left( \dot{m}_{CH_4;in;REF} \cdot (C_{p;CH_4;in;REF} \cdot (T_{in;REF} - T_0)) \right) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (54)$$

$$\dot{Q}_{H_2O;in;REF} = (\dot{m}_{H_2O;in;REF} \cdot C_{p;H_2O;in;REF} \cdot (T_{in;REF} - T_0)) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (55)$$

$$\dot{Q}_{CO_2;in;REF} = (\dot{m}_{CO_2;in;REF} \cdot C_{p;CO_2;in;REF} \cdot (T_{in;REF} - T_0)) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (56)$$

$$\delta\dot{Q}_{in;REF} = \dot{Q}_{CO_2;in;REF} + \dot{Q}_{H_2O;in;REF} + \dot{Q}_{CH_4;in;REF} \quad (57)$$

The heating of the inlet gas requires:

$$P_0 = P \cdot \left| 101,325000 \frac{\text{kPa}}{\text{atm}} \right| \quad (58)$$

The heat of the outlet gasses going to the SOFC

$$C_{p;CH_4;out;REF} = c_p \left( \text{Methane}; P = P_0; T = \left( \frac{T_{out;REF} + T_0}{2} \right) \right) \quad (59)$$

$$C_{p;H_2O;out;REF} = c_p \left( \text{Steam}; P = P_0; T = \left( \frac{T_{out;REF} + T_0}{2} \right) \right) \quad (60)$$

$$C_{p;CO_2;out;REF} = c_p \left( \text{CarbonDioxide}; P = P_0; T = \left( \frac{T_{out;REF} + T_0}{2} \right) \right) \quad (61)$$

$$C_{p;H_2;out;REF} = c_p \left( \text{Hydrogen}; P = P_0; T = \left( \frac{T_{out;REF} + T_0}{2} \right) \right) \quad (62)$$

$$C_{p;CO;out;REF} = c_p \left( \text{CarbonMonoxide}; P = P_0; T = \left( \frac{T_{out;REF} + T_0}{2} \right) \right) \quad (63)$$

$$\dot{Q}_{CH_4;out;REF} = \dot{m}_{CH_4;out;REF} \cdot ((C_{p;CH_4;out;REF} \cdot (T_{out;REF} - T_0))) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (64)$$

$$\dot{Q}_{H_2O;out;REF} = (\dot{m}_{H_2O;out;REF} \cdot C_{p;H_2O;out;REF} \cdot (T_{out;REF} - T_0)) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (65)$$

$$\dot{Q}_{CO_2;out;REF} = (\dot{m}_{CO_2;out;REF} \cdot C_{p;CO_2;out;REF} \cdot (T_{out;REF} - T_0)) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (66)$$

$$\dot{Q}_{CO;out;REF} = \dot{m}_{CO;out;REF} \cdot ((C_{p;CO;out;REF} \cdot (T_{out;REF} - T_0))) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (67)$$

$$\dot{Q}_{H_2;out;REF} = \dot{m}_{H_2;out;REF} \cdot ((C_{p;H_2;out;REF} \cdot (T_{out;REF} - T_0))) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (68)$$

$$\delta\dot{Q}_{out;REF} = \dot{Q}_{CH_4;out;REF} + \dot{Q}_{H_2O;out;REF} + \dot{Q}_{CO_2;out;REF} + \dot{Q}_{CO;out;REF} + \dot{Q}_{H_2;out;REF} \quad (69)$$

The heat of substances coming from the calciner

$$C_{p;850}^o = 52,22 \text{ [kJ/kmol}\cdot\text{K]} \quad (70)$$

$$C_{p;CaO;in;REF} = \frac{C_{p;850}^o}{MW(CaO)} \quad (71)$$

$$C_{p;MgO;in;REF} = 1,101 \text{ [kJ/kg}\cdot\text{K]} \quad (72)$$

$$C_{p;Catalyst;in;REF} = 1,072 \text{ [kJ/kg}\cdot\text{K]} \quad (73)$$

$$CaO_{per;CD} = 0,598 \quad (74)$$

$$\dot{m}_{MgO;in;REF} = \dot{m}_{CaO;in;REF} \cdot 0,4/CaO_{per;CD} \quad (75)$$

$$\dot{m}_{Catalyst;in;REF} = \frac{\dot{m}_{MgO;in;REF} + \dot{m}_{CaO;in;REF}}{2,8} \quad (76)$$

$$\dot{Q}_{MgO;in;REF} = \dot{m}_{MgO;in;REF} \cdot C_{p;MgO;in;REF} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (77)$$

$$\dot{Q}_{Catalyst;in;REF} = \dot{m}_{Catalyst;in;REF} \cdot C_{p;Catalyst;in;REF} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (78)$$

$$\dot{Q}_{CaO;in;REF} = \dot{m}_{CaO;in;REF} \cdot C_{p;CaO;in;REF} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (79)$$

$$\dot{Q}_{solids;in;REF} = \dot{Q}_{MgO;in;REF} + \dot{Q}_{Catalyst;in;REF} + \dot{Q}_{CaO;in;REF} \quad (80)$$

### The heat of substances going to the regenerator

$$C_{p;850;CaO}^o = 51,19 \text{ [kJ/kmol} \cdot \text{K]} \quad (81)$$

$$C_{p;CaO;out;REF} = \frac{C_{p;850;CaO}^o}{MW(CaO)} \quad (82)$$

$$C_{p;CaCO3;REF} = 1,058 \text{ [kJ/kg} \cdot \text{K]} \quad (83)$$

$$C_{p;MgO;out;REF} = 1,076 \text{ [kJ/kg} \cdot \text{K]} \quad (84)$$

$$C_{p;Catalyst;out;REF} = 1,006 \text{ [kJ/kg} \cdot \text{K]} \quad (85)$$

$$\dot{m}_{MgO;out;REF} = \dot{m}_{MgO;in;REF} \quad (86)$$

$$\dot{m}_{Catalyst;out;REF} = \dot{m}_{Catalyst;in;REF} \quad (87)$$

$$\dot{Q}_{MgO;out;REF} = \dot{m}_{MgO;out;REF} \cdot C_{p;MgO;out;REF} \cdot (T_{out;REF} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (88)$$

$$\dot{Q}_{Catalyst;out;REF} = \dot{m}_{Catalyst;out;REF} \cdot C_{p;Catalyst;out;REF} \cdot (T_{out;REF} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (89)$$

$$\dot{Q}_{CaCO3;out;REF} = \dot{m}_{CaCO3;out;REF} \cdot C_{p;CaCO3;REF} \cdot (T_{out;REF} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (90)$$

$$\dot{Q}_{CaO;out;REF} = \dot{m}_{CaO;out;REF} \cdot C_{p;CaO;out;REF} \cdot (T_{out;REF} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (91)$$

$$\dot{Q}_{solids;out;REF} = \dot{Q}_{MgO;out;REF} + \dot{Q}_{Catalyst;out;REF} + \dot{Q}_{CaCO3;out;REF} + \dot{Q}_{CaO;out;REF} \quad (92)$$

### Energy of the reaction

$$\Delta H_{rxn;SR} = 206 \text{ [kJ/mol]} \quad (93)$$

$$\Delta H_{rxn;WGS} = -41 \text{ [kJ/mol]} \quad (94)$$

$$\Delta H_{rxn;Carb} = -160 \text{ [kJ/mol]} \quad (95)$$



$$\Delta H_{rxn;Calc} = 160 \text{ [kJ/mol]} \quad (96)$$

$$\dot{Q}_{rxn;SR;REF} = \Delta H_{rxn;SR} \cdot x_1 \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (97)$$

$$\dot{Q}_{rxn;WGS;REF} = \Delta H_{rxn;WGS} \cdot x_2 \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (98)$$

$$\dot{Q}_{rxn;Carb;REF} = \Delta H_{rxn;Carb} \cdot x_3 \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (99)$$

$$\delta \dot{Q}_{rxn;REF} = \dot{Q}_{rxn;SR;REF} + \dot{Q}_{rxn;WGS;REF} + \dot{Q}_{rxn;Carb;REF} \quad (100)$$

### Energy Balance

$$loss = 0,00 \quad (101)$$

$$\dot{Q}_{loss;REF} = \left( \delta \dot{Q}_{in;REF} + \dot{Q}_{solids;in;REF} \right) \cdot loss \quad (102)$$

$$\delta \dot{Q}_{in;REF} + \dot{Q}_{solids;in;REF} = \delta \dot{Q}_{out;REF} + \dot{Q}_{solids;out;REF} + \delta \dot{Q}_{rxn;REF} + \dot{Q}_{loss;REF} \quad (103)$$

### Mass Balance

$$\dot{m}_{in;solids;REF} = \dot{m}_{CaO;in;REF} + \dot{m}_{MgO;in;REF} + \dot{m}_{Catalyst;in;REF} \quad (104)$$

$$\dot{m}_{in;REF} = \dot{m}_{CH_4;in;REF} + \dot{m}_{CO_2;in;REF} + \dot{m}_{H_2O;in;REF} \quad (105)$$

$$\dot{m}_{out;solids} = \dot{m}_{CaCO_3;out;REF} + \dot{m}_{MgO;out;REF} + \dot{m}_{Catalyst;out;REF} + \dot{m}_{CaO;out;REF} \quad (106)$$

$$\dot{m}_{out;REF} = \dot{m}_{CH_4;out;REF} + \dot{m}_{CO_2;out;REF} + \dot{m}_{CO;out;REF} + \dot{m}_{H_2;out;REF} + \dot{m}_{H_2O;out;REF} \quad (107)$$

$$\dot{m}_{in;REF} + \dot{m}_{in;solids;REF} = \dot{m}_{out;REF} + \dot{m}_{out;solids} \quad (108)$$

### The Regenerator!

#### The chemical equilibrium reactions in REG

$$\dot{n}_{gas;in;REG} = \dot{n}_{H_2O;in;REG} + \dot{n}_{H_2;in;REG} \quad (109)$$

$$\dot{n}_{H_2O;in;REG} = \dot{n}_{gas;in;REG} \cdot Comp_{H_2O;in;REG} \quad (110)$$

$$\dot{n}_{H_2;in;REG} = \dot{n}_{gas;in;REG} \cdot Comp_{H_2;in;REG} \quad (111)$$

$$\dot{n}_{gas;out;REG} = \dot{n}_{H_2;eq;REG} + \dot{n}_{H_2O;eq;REG} + \dot{n}_{CO_2;eq;REG} + \dot{n}_{CO;eq;REG} \quad (112)$$

$$\dot{n}_{CaCO_3;eq;REF} = x_{reg} \quad (113)$$

$$\dot{n}_{CO_2;eq;REG} = x_{reg} - x_4 \quad (114)$$

$$\dot{n}_{CaO;eq;REG} = \dot{n}_{CaO;eq;REF} + x_{reg} \quad (115)$$

$$\dot{n}_{CaCO_3;eq;REG} = \dot{n}_{CaCO_3;eq;REF} - x_{reg} \quad (116)$$

$$\dot{n}_{H_2;eq;REG} = \dot{n}_{H_2;in;REG} - x_4 \quad (117)$$

$$\dot{n}_{H_2O;eq;REG} = \dot{n}_{H_2O;in;REG} + x_4 \quad (118)$$

$$\dot{n}_{CO;eq;REG} = x_4 \quad (119)$$

$$\dot{n}_{tot;eq;REG} = \dot{n}_{H_2O;eq;REG} + \dot{n}_{H_2;eq;REG} + \dot{n}_{CO_2;eq;REG} + \dot{n}_{CO;eq;REG} \quad (120)$$

$$K_{p;WGS;REG} = \frac{1}{\exp\left(\left(4160 \frac{[K]}{T_{out;REG}}\right) - 3,798\right)} \quad (121)$$

$$K_{p;WGS;REG} = \frac{(\dot{n}_{H_2O;eq;REG}) \cdot (\dot{n}_{CO;eq;REG})}{(\dot{n}_{CO_2;eq;REG}) \cdot (\dot{n}_{H_2;eq;REG})} \quad (122)$$

$$T_{in;REG} = \text{ConvertTemp}(C; K; 750) \quad (123)$$

$$T_{out;REG} = \text{ConvertTemp}(C; K; 852) \quad (124)$$

$$T_{in;solids;REG} = \text{ConvertTemp}(C; K; 545) \quad (125)$$

$$Y_{H_2;out;REG} = 0,0066 \quad (126)$$

$$Y_{H_2O;out;REG} = 0,79 \quad (127)$$

$$Y_{H_2O;out;REG} = \dot{n}_{H_2O;eq;REG} / \dot{n}_{gas;out;REG} \quad (128)$$

$$Y_{H_2;out;REG} = \dot{n}_{H_2;eq;REG} / \dot{n}_{gas;out;REG} \quad (129)$$

$$Y_{CO_2;out;REG} = \dot{n}_{CO_2;eq;REG} / \dot{n}_{gas;out;REG} \quad (130)$$

$$Y_{CO;out;REG} = \dot{n}_{CO;eq;REG} / \dot{n}_{gas;out;REG} \quad (131)$$

### Energy Balance equations

$$\dot{m}_{CaCO_3;in;REG} = \dot{m}_{CaCO_3;out;REF} \quad (132)$$

$$\dot{m}_{CaO;in;REG} = \dot{m}_{CaO;out;REF} \quad (133)$$

$$\dot{m}_{MgO;in;REG} = \dot{m}_{MgO;out;REF} \quad (134)$$

$$\dot{m}_{Catalyst;in;REG} = \dot{m}_{Catalyst;out;REF} \quad (135)$$

$$\dot{m}_{H_2O;in;REG} = MW(H_2O) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{H_2O;in;REG} \quad (136)$$

$$\dot{m}_{H_2;in;REG} = MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{H_2;in;REG} \quad (137)$$

$$\dot{m}_{CO_2;out;REG} = MW(CO_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CO_2;eq;REG} \quad (138)$$

$$\dot{m}_{CaO;out;REG} = MW(CaO) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{CaO;eq;REG} \quad (139)$$

$$\dot{m}_{H_2O;out;REG} = MW(H_2O) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{H_2O;eq;REG} \quad (140)$$

$$\dot{m}_{H_2;out;REG} = MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \cdot \dot{n}_{H_2;eq;REG} \quad (141)$$

$$C_{p;H2O;in;REG} = c_p \left( \text{Steam}; P = P_0; T = \frac{T_{in;REG} + T_0}{2} \right) \quad (142)$$

$$C_{p;H2;in;REG} = c_p \left( \text{Hydrogen}; P = P_0; T = \frac{T_{in;REG} + T_0}{2} \right) \quad (143)$$

$$C_{p;H2O;out;REG} = c_p \left( \text{Steam}; P = P_0; T = \frac{T_{out;REG} + T_0}{2} \right) \quad (144)$$

$$C_{p;H2;out;REG} = c_p \left( \text{Hydrogen}; P = P_0; T = \frac{T_{out;REG} + T_0}{2} \right) \quad (145)$$

$$C_{p;CO2;out;REG} = c_p \left( \text{CarbonDioxide}; P = P_0; T = \frac{T_{out;REG} + T_0}{2} \right) \quad (146)$$

$$C_{p;CaO;in;REG} = C_{p;CaO;out;REF} \quad (147)$$

$$C_{p;CaO;out;REG} = C_{p;CaO;in;REF} \quad (148)$$

$$\dot{Q}_{in;MgO;REG} = \dot{m}_{MgO;in;REG} \cdot C_{p;MgO;out;REF} \cdot (T_{in;solids;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (149)$$

$$\dot{Q}_{in;Catalyst;REG} = \dot{m}_{Catalyst;in;REG} \cdot C_{p;Catalyst;out;REF} \cdot (T_{in;solids;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (150)$$

$$\dot{Q}_{in;CaCO3;REG} = \dot{m}_{CaCO3;in;REG} \cdot C_{p;CaCO3;REF} \cdot (T_{in;solids;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (151)$$

$$\dot{Q}_{in;CaO;REG} = \dot{m}_{CaO;in;REG} \cdot C_{p;CaO;in;REG} \cdot (T_{in;solids;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (152)$$

$$\dot{Q}_{in;H2;REG} = \dot{m}_{H2;in;REG} \cdot C_{p;H2;in;REG} \cdot (T_{in;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (153)$$

$$\dot{Q}_{in;H2O;REG} = \dot{m}_{H2O;in;REG} \cdot C_{p;H2O;in;REG} \cdot (T_{in;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (154)$$

$$\delta Q_{in;REG} = \dot{Q}_{in;H2;REG} + \dot{Q}_{in;H2O;REG} \quad (155)$$

$$\delta Q_{in;solids;REG} = \dot{Q}_{in;MgO;REG} + \dot{Q}_{in;Catalyst;REG} + \dot{Q}_{in;CaCO3;REG} + \dot{Q}_{in;CaO;REG} \quad (156)$$

$$\delta Q_{rxn;REG} = \Delta H_{rxn;Calc} \cdot x_{reg} \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (157)$$

$$\dot{Q}_{out;H2;REG} = \dot{m}_{H2;out;REG} \cdot C_{p;H2;out;REG} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (158)$$

$$\dot{Q}_{out;H2O;REG} = \dot{m}_{H2O;out;REG} \cdot C_{p;H2O;out;REG} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (159)$$

$$\dot{Q}_{out;CO2;REG} = \dot{m}_{CO2;out;REG} \cdot C_{p;CO2;out;REG} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (160)$$

$$\dot{Q}_{out;CaO;REG} = \dot{m}_{CaO;out;REG} \cdot C_{p;CaO;out;REG} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (161)$$

$$\dot{Q}_{out;MgO;REG} = \dot{m}_{MgO;in;REG} \cdot C_{p;MgO;in;REF} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (162)$$

$$\dot{Q}_{out;Catalyst;REG} = \dot{m}_{Catalyst;in;REG} \cdot C_{p;Catalyst;in;REF} \cdot (T_{out;REG} - T_0) \cdot \left| 1,000000000 \frac{\text{kW}}{\text{kJ/s}} \right| \quad (163)$$

$$\delta \dot{Q}_{out;solids;REG} = \dot{Q}_{out;CaO;REG} + \dot{Q}_{out;MgO;REG} + \dot{Q}_{out;Catalyst;REG} \quad (164)$$

$$\delta \dot{Q}_{out;REG} = \dot{Q}_{out;H2;REG} + \dot{Q}_{out;H2O;REG} + \dot{Q}_{out;CO2;REG} \quad (165)$$

$$Loss_{REG} = 0,0 \quad (166)$$

$$\dot{Q}_{loss;REG} = (\delta \dot{Q}_{in;REG} + \delta \dot{Q}_{in;solids;REG} + \Delta Q_{HEAT;NEED;REG}) \cdot Loss_{REG} \quad (167)$$

$$\Delta Q_{in;REG} = \delta \dot{Q}_{in;REG} + \delta \dot{Q}_{in;solids;REG} + \Delta Q_{HEAT;NEED;REG} \quad (168)$$

$$\Delta \dot{Q}_{out;REG} = \delta \dot{Q}_{out;solids;REG} + \delta \dot{Q}_{out;REG} + \delta \dot{Q}_{rxn;REG} + \dot{Q}_{loss;REG} \quad (169)$$

$$\Delta \dot{Q}_{in;REG} = \Delta \dot{Q}_{out;REG} \quad (170)$$

$$HydrogenPower_{REF} = LHV_{H2} \cdot \dot{m}_{H2;out;REF} \quad (171)$$

$$PowerOfHydrogen = LHV_{H2} \cdot \dot{m}_{H2;out;SOFC} \quad (172)$$

$$\eta_{CoGeneration} = \frac{LHV_{H2} \cdot \dot{m}_{H2;out;SOFC} + P_{SOFC}}{LHV_{CH4} \cdot (\dot{m}_{CH4;in;REF} + \dot{m}_{CH4;burner;in})} \quad (173)$$

$$\eta_{StandAlone} = LHV_{H2} \cdot \frac{\dot{m}_{H2;out;REF}}{LHV_{CH4} \cdot (\dot{m}_{CH4;in;REF} + \dot{m}_{CH4;burner;in})} \quad (174)$$

$$PowerOfMethane_{burner} = \dot{m}_{CH4;burner;in} \cdot LHV_{CH4} \quad (175)$$

$$PowerOfMethane = \dot{m}_{CH4;in;REF} \cdot LHV_{CH4} \quad (176)$$

### Burner!

$$\eta_{burner} = 0,98 \quad (177)$$

$$T_{in;burner} = \text{ConvertTemp}(C; K; 800) \quad (178)$$

$$T_{out;burner} = \text{ConvertTemp}(C; K; 1050) \quad (179)$$

$$T_{in;HeatExchanger} = T_{out;burner} \quad (180)$$

$$T_{out;HeatExchanger} = \text{ConvertTemp}(C; K; 860) \quad (181)$$

$$C_{p;air;HeatExchanger;in} = c_p \left( Air; T = \left( \left( \frac{T_{in;HeatExchanger} + T_0}{2} \right) \right) \right) \quad (182)$$

$$C_{p;air;HeatExchanger;out} = c_p \left( Air; T = \left( \left( \frac{T_{out;HeatExchanger} + T_0}{2} \right) \right) \right) \quad (183)$$

$$C_{p;air;burner;in} = c_p \left( Air; T = \left( \left( \frac{T_{in;burner} + T_0}{2} \right) \right) \right) \quad (184)$$

$$C_{p;air;burner;SOFC;in} = c_p \left( Air; T = \left( \left( \frac{T_{SOFC} + T_0}{2} \right) \right) \right) \quad (185)$$

$$C_{p;air;burner;out} = c_p \left( Air; T = \left( \left( \frac{T_{out;burner} + T_0}{2} \right) \right) \right) \quad (186)$$

$$\dot{Q}_{air;SOFC;in;Burner} = \dot{m}_{air;SOFC;in;Burner} \cdot C_{p;air;burner;SOFC;in} \cdot (T_{SOFC} - T_0) \quad (187)$$

$$\dot{Q}_{air;burner;in} = \dot{m}_{air;burner;in} \cdot C_{p,air;burner;in} \cdot (T_{in;burner} - T_0) \quad (188)$$

$$\dot{Q}_{CH4;burner;in} = \dot{m}_{CH4;burner;in} \cdot (LHV_{CH4}) \quad (189)$$

$$\left( \dot{Q}_{CH4;burner;in} + \dot{Q}_{air;burner;in} + \dot{Q}_{air;SOFC;in;Burner} \right) \cdot \eta_{burner} = \dot{Q}_{HeatExchanger;in} \quad (190)$$

$$\dot{Q}_{HeatExchanger;in} = \dot{m}_{HeatExchanger;in} \cdot C_{p,air;HeatExchanger;in} \cdot (T_{in;HeatExchanger} - T_0) \quad (191)$$

$$\dot{Q}_{HeatExchanger;out} = \dot{m}_{HeatExchanger;out} \cdot C_{p,air;HeatExchanger;out} \cdot (T_{out;HeatExchanger} - T_0) \quad (192)$$

$$\dot{Q}_{HeatExchanger;in} = \Delta Q_{HEAT;NEED;REG} + \dot{Q}_{HeatExchanger;out} \quad (193)$$

$$\dot{m}_{air;SOFC;in;Burner} = \dot{m}_{O2;out;SOFC} + \dot{m}_{N2;in;SOFC} \quad (194)$$

$$\dot{m}_{HeatExchanger;in} = \dot{m}_{HeatExchanger;out} \quad (195)$$

$$\dot{m}_{HeatExchanger;out} = \dot{m}_{air;burner;out} \quad (196)$$

$$\dot{m}_{air;burner;in} + \dot{m}_{air;SOFC;in;Burner} + \dot{m}_{CH4;burner;in} = \dot{m}_{air;burner;out} \quad (197)$$

### SOFC!

$$T_{in;SOFC} = \text{ConvertTemp}(C; K; 730) \quad (198)$$

$$T_{SOFC} = \text{ConvertTemp}(C; K; 830) \quad (199)$$

$$FU = 0,48 \quad \text{Fuel Utilization} \quad (200)$$

$$OU = 0,1 \quad \text{Oxygen utilization} \quad (201)$$

$$N2_{Air;comp} = 0,80 \quad (202)$$

$$O2_{Air;comp} = 0,20 \quad (203)$$

### Gas going in to the SOFC

$$\dot{n}_{H2;in;SOFC} = \dot{n}_{H2;eq;REF} \quad (204)$$

$$\dot{n}_{H2O;in;SOFC} = \dot{n}_{H2O;eq;REF} \quad (205)$$

$$\dot{n}_{CH4;in;SOFC} = \dot{n}_{CH4;eq;REF} \quad (206)$$

$$\dot{n}_{CO2;in;SOFC} = \dot{n}_{CO2;eq;REF} \quad (207)$$

$$\dot{n}_{CO;in;SOFC} = \dot{n}_{CO;eq;REF} \quad (208)$$

$$\dot{n}_{H2;eq;SOFC} = \dot{n}_{H2;in;SOFC} + 3 \cdot x_{1;sofc} + x_{2;sofc} \quad (209)$$

$$\dot{n}_{H2O;eq;SOFC} = \dot{n}_{H2O;in;SOFC} - x_{1;sofc} - x_{2;sofc} \quad (210)$$

$$\dot{n}_{CH4;eq;SOFC} = \dot{n}_{CH4;in;SOFC} - x_{1;sofc} \quad (211)$$

$$\dot{n}_{CO2;eq;SOFC} = \dot{n}_{CO2;in;SOFC} + x_{2;sofc} \quad (212)$$

$$\dot{n}_{CO;eq;SOFC} = \dot{n}_{CO;in;SOFC} + x_{1;sofc} - x_{2;sofc} \quad (213)$$

$$\dot{n}_{tot;SOFC} = \dot{n}_{H2;in;SOFC} + \dot{n}_{H2O;in;SOFC} + \dot{n}_{CH4;in;SOFC} + \dot{n}_{CO2;in;SOFC} + \dot{n}_{CO;in;SOFC} + 2 \cdot x_{1;sofc} \quad (214)$$

$$K_{p,SR;SOFC} = \exp \left( \left( -26830 \frac{[K]}{T_{SOFC}} \right) + 30,11 \right) \cdot 1 \text{ [atm}^2\text{]} \quad (215)$$

$$K_{p,SR;SOFC} = \frac{\dot{n}_{CO;eq;SOFC} \cdot (\dot{n}_{H_2;eq;SOFC}^3) \cdot P^2}{\dot{n}_{CH_4;eq;SOFC} \cdot \dot{n}_{H_2O;eq;SOFC} \cdot (\dot{n}_{tot;SOFC})^2} \quad (216)$$

$$K_{p,WGS;SOFC} = \left( \exp \left( \left( 4160 \frac{[K]}{T_{SOFC}} \right) - 3,798 \right) \right) \quad (217)$$

$$K_{p,WGS;SOFC} = \left( \frac{(\dot{n}_{CO_2;eq;SOFC}) \cdot (\dot{n}_{H_2;eq;SOFC})}{\dot{n}_{H_2O;eq;SOFC} \cdot \dot{n}_{CO;eq;SOFC}} \right) \quad (218)$$

$$\dot{n}_{O_2;rxn;SOFC} = \left( \frac{\dot{m}_{H_2;SOFC} \cdot FU}{MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right|} \right) \cdot 0,5 \quad (219)$$

$$\dot{n}_{O_2;SOFC} = \dot{n}_{O_2;rxn;SOFC} / OU \quad (220)$$

$$\dot{n}_{N_2;SOFC} = (N_{2Air;comp} / O_{2Air;comp}) \cdot \dot{n}_{O_2;SOFC} \quad (221)$$

$$\dot{n}_{cat;tot;in} = \dot{n}_{O_2;SOFC} + \dot{n}_{N_2;SOFC} \quad (222)$$

$$\dot{m}_{H_2;in;SOFC} = \dot{n}_{H_2;in;SOFC} \cdot \left( MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (223)$$

$$\dot{m}_{H_2O;in;SOFC} = \dot{n}_{H_2O;in;SOFC} \cdot \left( MW(H_2O) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (224)$$

$$\dot{m}_{CH_4;in;SOFC} = \dot{n}_{CH_4;in;SOFC} \cdot \left( MW(CH_4) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (225)$$

$$\dot{m}_{CO_2;in;SOFC} = \dot{n}_{CO_2;in;SOFC} \cdot \left( MW(CO_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (226)$$

$$\dot{m}_{CO;in;SOFC} = \dot{n}_{CO;in;SOFC} \cdot \left( MW(CO) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (227)$$

$$\dot{m}_{O_2;in;SOFC} = \dot{n}_{O_2;SOFC} \cdot \left( MW(O_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (228)$$

$$\dot{m}_{N_2;in;SOFC} = \dot{n}_{N_2;SOFC} \cdot \left( MW(N_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (229)$$

$$AirFlowCathode = \dot{m}_{O_2;in;SOFC} + \dot{m}_{N_2;in;SOFC} \quad (230)$$

$$\dot{n}_{H_2O;rxn;SOFC} = \frac{\dot{m}_{H_2;SOFC} \cdot FU}{MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right|} \quad (231)$$

$$\dot{m}_{H_2;SOFC} = \dot{n}_{H_2;eq;SOFC} \cdot \left( MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (232)$$

$$\dot{m}_{H_2O;SOFC} = (\dot{n}_{H_2O;eq;SOFC} + \dot{n}_{H_2O;rxn;SOFC}) \cdot \left( MW(H_2O) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (233)$$

$$\dot{m}_{CH_4;SOFC} = \dot{n}_{CH_4;eq;SOFC} \cdot \left( MW(CH_4) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (234)$$

$$\dot{m}_{CO_2;SOFC} = \dot{n}_{CO_2;eq;SOFC} \cdot \left( MW(CO_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (235)$$

$$\dot{m}_{CO;SOFC} = \dot{n}_{CO;eq;SOFC} \cdot \left( MW(CO) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (236)$$

$$\dot{m}_{O_2;out;SOFC} = (\dot{n}_{O_2;SOFC} - \dot{n}_{O_2;rxn;SOFC}) \cdot \left( MW(O_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right| \right) \quad (237)$$

$$\dot{m}_{H_2;out;SOFC} = \dot{m}_{H_2;SOFC} \cdot (1 - FU) \quad (238)$$

$$\dot{n}_{H_2;out;SOFC} = \left( \frac{\dot{m}_{H_2;out;SOFC}}{MW(H_2) \cdot \left| 0,001000000 \frac{\text{kg/mol}}{\text{kg/kmol}} \right|} \right) \quad (239)$$

$$C_{p;H_2;SOFC} = c_p \left( \text{Hydrogen}; P = P_0; T = \frac{T_{in;SOFC} + T_0}{2} \right) \quad (240)$$

$$C_{p;H_2O;SOFC} = c_p \left( \text{Steam}; P = P_0; T = \frac{T_{in;SOFC} + T_0}{2} \right) \quad (241)$$

$$C_{p;CH_4;SOFC} = c_p \left( \text{Methane}; P = P_0; T = \frac{T_{in;SOFC} + T_0}{2} \right) \quad (242)$$

$$C_{p;CO_2;SOFC} = c_p \left( \text{CarbonDioxide}; P = P_0; T = \frac{T_{in;SOFC} + T_0}{2} \right) \quad (243)$$

$$C_{p;CO;SOFC} = c_p \left( \text{CarbonMonoxide}; P = P_0; T = \frac{T_{in;SOFC} + T_0}{2} \right) \quad (244)$$

$$C_{p;O_2;SOFC} = c_p \left( \text{Oxygen}; P = P_0; T = \frac{T_{in;cat;SOFC} + T_0}{2} \right) \quad (245)$$

$$C_{p;N_2;SOFC} = c_p \left( \text{Nitrogen}; P = P_0; T = \frac{T_{in;cat;SOFC} + T_0}{2} \right) \quad (246)$$

$$\dot{Q}_{H_2;in;SOFC} = \dot{m}_{H_2;in;SOFC} \cdot ((C_{p;H_2;SOFC} \cdot (T_{in;SOFC} - T_0))) \quad (247)$$

$$\dot{Q}_{H_2O;in;SOFC} = \dot{m}_{H_2O;in;SOFC} \cdot C_{p;H_2O;SOFC} \cdot (T_{in;SOFC} - T_0) \quad (248)$$

$$\dot{Q}_{CH_4;in;SOFC} = \dot{m}_{CH_4;in;SOFC} \cdot ((C_{p;CH_4;SOFC} \cdot (T_{in;SOFC} - T_0))) \quad (249)$$

$$\dot{Q}_{CO_2;in;SOFC} = \dot{m}_{CO_2;in;SOFC} \cdot C_{p;CO_2;SOFC} \cdot (T_{in;SOFC} - T_0) \quad (250)$$

$$\dot{Q}_{CO;in;SOFC} = \dot{m}_{CO;in;SOFC} \cdot ((C_{p;CO;SOFC} \cdot (T_{in;SOFC} - T_0))) \quad (251)$$

$$\dot{Q}_{O_2;in;cat;SOFC} = \dot{m}_{O_2;in;SOFC} \cdot C_{p;O_2;SOFC} \cdot (T_{in;cat;SOFC} - T_0) \quad (252)$$

$$\dot{Q}_{N_2;in;cat;SOFC} = \dot{m}_{N_2;in;SOFC} \cdot C_{p;N_2;SOFC} \cdot (T_{in;cat;SOFC} - T_0) \quad (253)$$

$$\Delta Q_{in;SOFC} = \dot{Q}_{O_2;in;cat;SOFC} + \dot{Q}_{N_2;in;cat;SOFC} + \dot{Q}_{H_2;in;SOFC} + \dot{Q}_{H_2O;in;SOFC} + \dot{Q}_{CH_4;in;SOFC} + \dot{Q}_{CO_2;in;SOFC} + \dot{Q}_{CO;in;SOFC} \quad (254)$$

$$\dot{Q}_{SR;rxn;SOFC} = \Delta H_{rxn;SR} \cdot x_{1;sofc} \quad (255)$$

$$\dot{Q}_{WGS;rxn;SOFC} = \Delta H_{rxn;WGS} \cdot x_{2;sofc} \quad (256)$$

$$\dot{Q}_{H2;rxn;SOFC} = -FU \cdot \dot{m}_{H2;SOFC} \cdot LHV_{H2} \quad (257)$$

$$\Delta Q_{rxn;SOFC} = \dot{Q}_{SR;rxn;SOFC} + \dot{Q}_{WGS;rxn;SOFC} + \dot{Q}_{H2;rxn;SOFC} \quad (258)$$

$$C_{p;H2;SOFC;out} = c_p \left( \text{Hydrogen}; P = P_0; T = \frac{T_{SOFC} + T_0}{2} \right) \quad (259)$$

$$C_{p;H2O;SOFC;out} = c_p \left( \text{Steam}; P = P_0; T = \frac{T_{SOFC} + T_0}{2} \right) \quad (260)$$

$$C_{p;CH4;SOFC;out} = c_p \left( \text{Methane}; P = P_0; T = \frac{T_{SOFC} + T_0}{2} \right) \quad (261)$$

$$C_{p;CO2;SOFC;out} = c_p \left( \text{CarbonDioxide}; P = P_0; T = \frac{T_{SOFC} + T_0}{2} \right) \quad (262)$$

$$C_{p;CO;SOFC;out} = c_p \left( \text{CarbonMonoxide}; P = P_0; T = \frac{T_{SOFC} + T_0}{2} \right) \quad (263)$$

$$C_{p;O2;SOFC;out} = c_p \left( \text{Oxygen}; P = P_0; T = \frac{T_{SOFC} + T_0}{2} \right) \quad (264)$$

$$C_{p;N2;SOFC;out} = c_p \left( \text{Nitrogen}; P = P_0; T = \frac{T_{SOFC} + T_0}{2} \right) \quad (265)$$

$$\dot{Q}_{H2;out;SOFC} = \dot{m}_{H2;out;SOFC} \cdot ((C_{p;H2;SOFC;out} \cdot (T_{SOFC} - T_0))) \quad (266)$$

$$\dot{Q}_{H2O;out;SOFC} = \dot{m}_{H2O;SOFC} \cdot C_{p;H2O;SOFC;out} \cdot (T_{SOFC} - T_0) \quad (267)$$

$$\dot{Q}_{CH4;out;SOFC} = \dot{m}_{CH4;SOFC} \cdot ((C_{p;CH4;SOFC;out} \cdot (T_{SOFC} - T_0))) \quad (268)$$

$$\dot{Q}_{CO2;out;SOFC} = \dot{m}_{CO2;SOFC} \cdot C_{p;CO2;SOFC;out} \cdot (T_{SOFC} - T_0) \quad (269)$$

$$\dot{Q}_{CO;out;SOFC} = \dot{m}_{CO;SOFC} \cdot ((C_{p;CO;SOFC;out} \cdot (T_{SOFC} - T_0))) \quad (270)$$

$$\dot{Q}_{O2;out;SOFC} = \dot{m}_{O2;out;SOFC} \cdot C_{p;O2;SOFC;out} \cdot (T_{SOFC} - T_0) \quad (271)$$

$$\dot{Q}_{N2;out;SOFC} = \dot{m}_{N2;in;SOFC} \cdot C_{p;N2;SOFC;out} \cdot (T_{SOFC} - T_0) \quad (272)$$

$$\Delta Q_{out;SOFC} = \dot{Q}_{O2;out;SOFC} + \dot{Q}_{N2;out;SOFC} + \dot{Q}_{H2;out;SOFC} + \dot{Q}_{H2O;out;SOFC} + \dot{Q}_{CH4;out;SOFC} + \dot{Q}_{CO2;out;SOFC} + \dot{Q}_{CO;out;SOFC} \quad (273)$$

$$\text{HeatGenerated} = ((\dot{m}_{H2;SOFC} \cdot LHV_{H2} \cdot FU) - P_{SOFC}) \quad (274)$$

$$\text{HeatLoss} = 0,05 \quad (275)$$

$$\dot{Q}_{loss;SOFC} = P_{SOFC} \cdot \text{HeatLoss} \quad (276)$$

$$\Delta Q_{in;SOFC} = \Delta Q_{out;SOFC} + \Delta Q_{rxn;SOFC} + \dot{Q}_{loss;SOFC} + P_{SOFC} \quad (277)$$

$$n_{total;cells} = I_{FC} / I_{Cell} \quad (278)$$

$$\text{Faraday} = F\# \cdot \left| 0,001000000 \frac{\text{coulomb/mol}}{\text{coulomb/kmol}} \right| \quad (279)$$

$$I_{FC} = \left( (2 \cdot \text{Faraday}) \cdot FU \cdot \dot{n}_{H2;eq;SOFC} \cdot \left| 1,000000000 \frac{\text{A}}{\text{Coulomb/s}} \right| \right) \quad (280)$$



$$P_{SOFC} = V_{FC;Cell} \cdot I_{FC} \cdot \left| 0,001000000 \frac{\text{kW}}{\text{W}} \right| \cdot 0,95 \quad (281)$$

$$P_{H2} = \dot{n}_{H2;eq;SOFC} / \dot{n}_{tot;SOFC} \quad (282)$$

$$P_{O2} = \dot{n}_{O2;SOFC} / \dot{n}_{cat;tot;in} \quad (283)$$

$$P_{H2O} = \dot{n}_{H2O;eq;SOFC} / \dot{n}_{tot;SOFC} \quad (284)$$

$$E^0 = 1,253 \text{ [V]} - 2,4516 \text{ [V/K]} \cdot 10^{-4} \cdot T_{SOFC} \quad (285)$$

$$V_{nernst} = E^0 + \left( \frac{R\# \cdot T_{SOFC}}{2 \cdot F\#} \right) \cdot \ln \left( \left( \frac{P_{H2} \cdot P_{O2}^{0,5}}{P_{H2O}} \right) \right) \cdot \left| 1000,00000 \frac{\text{J/coulomb}}{\text{kJ/coulomb}} \right| \quad (286)$$

$$J_{FC;Cell} = 0,290 \text{ [A/cm}^2\text{]} \quad (287)$$

$$r_{Cell} = 0,348 \text{ [Ohm} \cdot \text{cm}^2\text{]} \quad (288)$$

$$V_{tot} = J_{FC;Cell} \cdot r_{Cell} \quad (289)$$

$$V_{FC;Cell} = V_{nernst} - V_{tot} \quad (290)$$

$$I_{Cell} = 127 \text{ [cm}^2\text{]} \cdot J_{FC;Cell} \quad (291)$$

$$\dot{n}_{tot;out;SOFC} = \dot{n}_{H2;out;SOFC} + \dot{n}_{CH4;eq;SOFC} + \dot{n}_{CO2;eq;SOFC} + \dot{n}_{CO;eq;SOFC} \quad (292)$$

$$Y_{H2;out;dry;SOFC} = \dot{n}_{H2;out;SOFC} / \dot{n}_{tot;out;SOFC} \quad (293)$$

$$Y_{CH4;out;dry;SOFC} = \dot{n}_{CH4;eq;SOFC} / \dot{n}_{tot;out;SOFC} \quad (294)$$

$$Y_{CO2;out;dry;SOFC} = \dot{n}_{CO2;eq;SOFC} / \dot{n}_{tot;out;SOFC} \quad (295)$$

$$Y_{CO;out;dry;SOFC} = \dot{n}_{CO;eq;SOFC} / \dot{n}_{tot;out;SOFC} \quad (296)$$

$$\dot{m}_{in;SOFC} = \dot{m}_{H2;in;SOFC} + \dot{m}_{H2O;in;SOFC} + \dot{m}_{CH4;in;SOFC} + \dot{m}_{CO2;in;SOFC} + \dot{m}_{CO;in;SOFC} + \dot{m}_{O2;in;SOFC} + \dot{m}_{N2;in;SOFC} \quad (297)$$

$$\dot{m}_{out;SOFC} = \dot{m}_{H2;out;SOFC} + \dot{m}_{H2O;SOFC} + \dot{m}_{CH4;SOFC} + \dot{m}_{CO2;SOFC} + \dot{m}_{CO;SOFC} + \dot{m}_{O2;out;SOFC} + \dot{m}_{N2;in;SOFC} \quad (298)$$

# Appendix C

## Solution for simulation of BioZEG

$$AirFlowCathode = 0,05435 \text{ [kg/s]}$$

$$CH4 = 0,95$$

$$Comp_{H2O;in;REG} = 0,9802$$

$$C_{p;air;burner;in} = 1,071 \text{ [kJ/kg-K]}$$

$$C_{p;air;burner;SOFC;in} = 1,075 \text{ [kJ/kg-K]}$$

$$C_{p;air;HeatExchanger;out} = 1,079 \text{ [kJ/kg-K]}$$

$$C_{p;CaO;in;REF} = 0,9312 \text{ [kJ/K-kg]}$$

$$C_{p;CaO;out;REF} = 0,9128 \text{ [kJ/K-kg]}$$

$$C_{p;Catalyst;in;REF} = 1,072 \text{ [kJ/kg-K]}$$

$$C_{p;CH4;in;REF} = 2,489 \text{ [kJ/kg-K]}$$

$$C_{p;CH4;SOFC} = 3,456 \text{ [kJ/kg-K]}$$

$$C_{p;CO2;in;REF} = 0,9309 \text{ [kJ/kg-K]}$$

$$C_{p;CO2;out;REG} = 1,132 \text{ [kJ/kg-K]}$$

$$C_{p;CO2;SOFC;out} = 1,127 \text{ [kJ/kg-K]}$$

$$C_{p;CO;SOFC} = 1,042 \text{ [kJ/kg-K]}$$

$$C_{p;H2O;in;REF} = 2,016 \text{ [kJ/kg-K]}$$

$$C_{p;H2O;out;REF} = 2,02 \text{ [kJ/kg-K]}$$

$$C_{p;H2O;SOFC} = 2,057 \text{ [kJ/kg-K]}$$

$$C_{p;H2;in;REG} = 14,58 \text{ [kJ/kg-K]}$$

$$C_{p;H2;out;REG} = 14,62 \text{ [kJ/kg-K]}$$

$$C_{p;H2;SOFC;out} = 14,61 \text{ [kJ/kg-K]}$$

$$C_{p;MgO;out;REF} = 1,076 \text{ [kJ/kg-K]}$$

$$C_{p;N2;SOFC;out} = 1,098 \text{ [kJ/kg-K]}$$

$$C_{p;O2;SOFC;out} = 1,028 \text{ [kJ/kg-K]}$$

$$C_{p;850;CaO}^o = 51,19 \text{ [kJ/kmol-K]}$$

$$\Delta H_{rxn;Carb} = -160 \text{ [kJ/mol]}$$

$$\Delta H_{rxn;WGS} = -41 \text{ [kJ/mol]}$$

$$\delta \dot{Q}_{in;REF} = 1,317 \text{ [kW]}$$

$$\Delta \dot{Q}_{in;SOFC} = 47,76 \text{ [kW]}$$

$$\delta \dot{Q}_{out;REF} = 4,38 \text{ [kW]}$$

$$\Delta \dot{Q}_{out;SOFC} = 53,12 \text{ [kW]}$$

$$\delta \dot{Q}_{rxn;REF} = 0,1928 \text{ [kW]}$$

$$\Delta \dot{Q}_{rxn;SOFC} = -18,06 \text{ [kW]}$$

$$\Delta Q_{out;REG} = 23,26 \text{ [kW]}$$

$$\eta_{CoGeneration} = 0,65$$

$$E^0 = 0,9826 \text{ [V]}$$

$$FU = 0,48$$

$$HeatLoss = 0,05$$

$$I_{Cell} = 36,83 \text{ [A]}$$

$$J_{FC;Cell} = 0,29 \text{ [A/cm}^2\text{]}$$

$$K_{p;SR} = 0,5391 \text{ [atm}^2\text{]}$$

$$K_{p;WGS} = 2,628$$

$$K_{p;WGS;SOFC} = 0,9734$$

$$LHV_{CO} = 10000 \text{ [kJ/kg]}$$

$$loss = 0$$

$$\dot{m}_{air;burner;in} = 0,0005748 \text{ [kg/s]}$$

$$\dot{m}_{air;SOFC;in;Burner} = 0,05314 \text{ [kg/s]}$$

$$\dot{m}_{CaCO3;out;REF} = 0,003899 \text{ [kg/s]}$$

$$\dot{m}_{CaO;in;REG} = 0,005097 \text{ [kg/s]}$$

$$\dot{m}_{CaO;out;REG} = 0,007282 \text{ [kg/s]}$$

$$\dot{m}_{Catalyst;in;REG} = 0,004284 \text{ [kg/s]}$$

$$CaO_{per;CD} = 0,618$$

$$CO2 = 0,04$$

$$Comp_{H2;in;REG} = 0,01978$$

$$C_{p;air;burner;out} = 1,101 \text{ [kJ/kg-K]}$$

$$C_{p;air;HeatExchanger;in} = 1,101 \text{ [kJ/kg-K]}$$

$$C_{p;CaCO3;REF} = 1,058 \text{ [kJ/kg-K]}$$

$$C_{p;CaO;in;REG} = 0,9128 \text{ [kJ/K-kg]}$$

$$C_{p;CaO;out;REG} = 0,9312 \text{ [kJ/K-kg]}$$

$$C_{p;Catalyst;out;REF} = 1,006 \text{ [kJ/kg-K]}$$

$$C_{p;CH4;out;REF} = 3,22 \text{ [kJ/kg-K]}$$

$$C_{p;CH4;SOFC;out} = 3,631 \text{ [kJ/kg-K]}$$

$$C_{p;CO2;out;REF} = 1,068 \text{ [kJ/kg-K]}$$

$$C_{p;CO2;SOFC} = 1,103 \text{ [kJ/kg-K]}$$

$$C_{p;CO;out;REF} = 1,041 \text{ [kJ/kg-K]}$$

$$C_{p;CO;SOFC;out} = 1,043 \text{ [kJ/kg-K]}$$

$$C_{p;H2O;in;REG} = 2,063 \text{ [kJ/kg-K]}$$

$$C_{p;H2O;out;REG} = 2,094 \text{ [kJ/kg-K]}$$

$$C_{p;H2O;SOFC;out} = 2,087 \text{ [kJ/kg-K]}$$

$$C_{p;H2;out;REF} = 14,54 \text{ [kJ/kg-K]}$$

$$C_{p;H2;SOFC} = 14,58 \text{ [kJ/kg-K]}$$

$$C_{p;MgO;in;REF} = 1,101 \text{ [kJ/kg-K]}$$

$$C_{p;N2;SOFC} = 1,089 \text{ [kJ/kg-K]}$$

$$C_{p;O2;SOFC} = 1,018 \text{ [kJ/kg-K]}$$

$$C_{p;850}^o = 52,22 \text{ [kJ/kmol-K]}$$

$$\Delta H_{rxn;Calc} = 160 \text{ [kJ/mol]}$$

$$\Delta H_{rxn;SR} = 206 \text{ [kJ/mol]}$$

$$\Delta \dot{Q}_{HEAT;NEED;REG} = 12,31 \text{ [kW]}$$

$$\delta \dot{Q}_{in;REG} = 1,503 \text{ [kW]}$$

$$\delta \dot{Q}_{in;solids;REG} = 9,443 \text{ [kW]}$$

$$\delta \dot{Q}_{out;REG} = 3,33 \text{ [kW]}$$

$$\delta \dot{Q}_{out;solids;REG} = 13,7 \text{ [kW]}$$

$$\delta \dot{Q}_{rxn;REG} = 6,233 \text{ [kW]}$$

$$\Delta Q_{in;REG} = 23,26 \text{ [kW]}$$

$$\eta_{burner} = 0,98$$

$$\eta_{StandAlone} = 0,76$$

$$Faraday = 96487 \text{ [Coulomb/mol]}$$

$$HeatGenerated = 6,153 \text{ [kW]}$$

$$HydrogenPowerREF = 37,38 \text{ [kW]}$$

$$I_{FC} = 14562 \text{ [A]}$$

$$K_{p;CO2} = 2,693 \text{ [1/kPa]}$$

$$K_{p;SR;SOFC} = 326,6 \text{ [atm}^2\text{]}$$

$$K_{p;WGS;REG} = 1,106$$

$$LHV_{CH4} = 52000 \text{ [kJ/kg]}$$

$$LHV_{H2} = 120000 \text{ [kJ/kg]}$$

$$Loss_{REG} = 0$$

$$\dot{m}_{air;burner;out} = 0,05402 \text{ [kg/s]}$$

$$\dot{m}_{CaCO3;in;REG} = 0,003899 \text{ [kg/s]}$$

$$\dot{m}_{CaO;in;REF} = 0,007282 \text{ [kg/s]}$$

$$\dot{m}_{CaO;out;REF} = 0,005097 \text{ [kg/s]}$$

$$\dot{m}_{Catalyst;in;REF} = 0,004284 \text{ [kg/s]}$$

$$\dot{m}_{Catalyst;out;REF} = 0,004284 \text{ [kg/s]}$$

$$\begin{aligned}
\dot{m}_{CH_4;burner;in} &= 0,0003028 \text{ [kg/s]} \\
\dot{m}_{CH_4;in;SOFC} &= 0,00001477 \text{ [kg/s]} \\
\dot{m}_{CH_4;SOFC} &= 6,553 \times 10^{-8} \text{ [kg/s]} \\
\dot{m}_{CO_2;in;SOFC} &= 0,00003852 \text{ [kg/s]} \\
\dot{m}_{CO_2;out;REG} &= 0,001693 \text{ [kg/s]} \\
\dot{m}_{CO;in;SOFC} &= 0,0000176 \text{ [kg/s]} \\
\dot{m}_{CO;SOFC} &= 0,00004514 \text{ [kg/s]} \\
\dot{m}_{H_2O;in;REG} &= 0,0009896 \text{ [kg/s]} \\
\dot{m}_{H_2O;out;REF} &= 0,001475 \text{ [kg/s]} \\
\dot{m}_{H_2O;SOFC} &= 0,00282 \text{ [kg/s]} \\
\dot{m}_{H_2;in;SOFC} &= 0,0003115 \text{ [kg/s]} \\
\dot{m}_{H_2;out;REG} &= 0,000001264 \text{ [kg/s]} \\
\dot{m}_{H_2;SOFC} &= 0,0003169 \text{ [kg/s]} \\
\dot{m}_{HeatExchanger;out} &= 0,05402 \text{ [kg/s]} \\
\dot{m}_{in;SOFC} &= 0,05621 \text{ [kg/s]} \\
\dot{m}_{MgO;in;REF} &= 0,004713 \text{ [kg/s]} \\
\dot{m}_{MgO;out;REF} &= 0,004713 \text{ [kg/s]} \\
\dot{m}_{O_2;in;SOFC} &= 0,01207 \text{ [kg/s]} \\
\dot{m}_{out;REF} &= 0,001858 \text{ [kg/s]} \\
\dot{m}_{out;solids} &= 0,01799 \text{ [kg/s]} \\
m_{solids;out;REF} &= 0,01799 \text{ [kg/s]} \\
\dot{n}_{CaCO_3;eq;REF} &= 0,03896 \text{ [mol/s]} \\
\dot{n}_{CaCO_3;out;REF} &= 0,03896 \text{ [mol/s]} \\
\dot{n}_{CaO;eq;REG} &= 0,1299 \text{ [mol/s]} \\
\dot{n}_{cat;tot;in} &= 1,887 \text{ [mol/s]} \\
\dot{n}_{CH_4;eq;SOFC} &= 0,00004085 \text{ [mol/s]} \\
\dot{n}_{CH_4;in;SOFC} &= 0,0009207 \text{ [mol/s]} \\
\dot{n}_{CO_2;eq;REG} &= 0,03848 \text{ [mol/s]} \\
\dot{n}_{CO_2;in;REF} &= 0,001672 \text{ [mol/s]} \\
\dot{n}_{CO;eq;REF} &= 0,0006284 \text{ [mol/s]} \\
\dot{n}_{CO;eq;SOFC} &= 0,001612 \text{ [mol/s]} \\
\dot{n}_{gas;in;REG} &= 0,05604 \text{ [mol/s]} \\
\dot{n}_{H_2O;eq;REF} &= 0,08189 \text{ [mol/s]} \\
\dot{n}_{H_2O;eq;SOFC} &= 0,08104 \text{ [mol/s]} \\
\dot{n}_{H_2O;in;REG} &= 0,05493 \text{ [mol/s]} \\
\dot{n}_{H_2O;rxn;SOFC} &= 0,07546 \text{ [mol/s]} \\
\dot{n}_{H_2;eq;REG} &= 0,000627 \text{ [mol/s]} \\
\dot{n}_{H_2;in;REG} &= 0,001108 \text{ [mol/s]} \\
\dot{n}_{H_2;out;SOFC} &= 0,08175 \text{ [mol/s]} \\
\dot{n}_{O_2;rxn;SOFC} &= 0,03773 \text{ [mol/s]} \\
\dot{n}_{tot;dry;REF} &= 0,157 \text{ [mol/s]} \\
\dot{n}_{tot;eq;REG} &= 0,095 \text{ [mol/s]} \\
\dot{n}_{tot;out;SOFC} &= 0,08417 \text{ [mol/s]} \\
n_{total;cells} &= 395,4 \\
OU &= 0,1 \\
PowerOfHydrogen &= 19,78 \text{ [kW]} \\
PowerOfMethane_{burner} &= 15,75 \text{ [kW]} \\
P_{H_2} &= 0,6532 \\
P_{O_2} &= 0,2 \\
\dot{Q}_{air;burner;in} &= 0,4772 \text{ [kW]} \\
\dot{Q}_{CaCO_3;out;REF} &= 2,372 \text{ [kW]} \\
\dot{Q}_{CaO;out;REF} &= 2,675 \text{ [kW]} \\
\dot{Q}_{Catalyst;out;REF} &= 2,478 \text{ [kW]}
\end{aligned}$$

$$\begin{aligned}
\dot{m}_{CH_4;in;REF} &= 0,0006371 \text{ [kg/s]} \\
\dot{m}_{CH_4;out;REF} &= 0,00001477 \text{ [kg/s]} \\
\dot{m}_{CO_2;in;REF} &= 0,00007358 \text{ [kg/s]} \\
\dot{m}_{CO_2;out;REF} &= 0,00003852 \text{ [kg/s]} \\
\dot{m}_{CO_2;SOFC} &= 0,00003559 \text{ [kg/s]} \\
\dot{m}_{CO;out;REF} &= 0,0000176 \text{ [kg/s]} \\
\dot{m}_{H_2O;in;REF} &= 0,002862 \text{ [kg/s]} \\
\dot{m}_{H_2O;in;SOFC} &= 0,001475 \text{ [kg/s]} \\
\dot{m}_{H_2O;out;REG} &= 0,0009983 \text{ [kg/s]} \\
\dot{m}_{H_2;in;REG} &= 0,000002235 \text{ [kg/s]} \\
\dot{m}_{H_2;out;REF} &= 0,0003115 \text{ [kg/s]} \\
\dot{m}_{H_2;out;SOFC} &= 0,0001648 \text{ [kg/s]} \\
\dot{m}_{HeatExchanger;in} &= 0,05402 \text{ [kg/s]} \\
\dot{m}_{in;REF} &= 0,003572 \text{ [kg/s]} \\
\dot{m}_{in;solids;REF} &= 0,01628 \text{ [kg/s]} \\
\dot{m}_{MgO;in;REG} &= 0,004713 \text{ [kg/s]} \\
\dot{m}_{N_2;in;SOFC} &= 0,04228 \text{ [kg/s]} \\
\dot{m}_{O_2;out;SOFC} &= 0,01087 \text{ [kg/s]} \\
\dot{m}_{out;SOFC} &= 0,05621 \text{ [kg/s]} \\
m_{solids;in;REF} &= 0,01628 \text{ [kg/s]} \\
N_{2Air;comp} &= 0,8 \\
\dot{n}_{CaCO_3;eq;REG} &= 0 \text{ [mol/s]} \\
\dot{n}_{CaO;eq;REF} &= 0,09089 \text{ [mol/s]} \\
\dot{n}_{CaO;in;REF} &= 0,1299 \text{ [mol/s]} \\
\dot{n}_{CH_4;eq;REF} &= 0,0009207 \text{ [mol/s]} \\
\dot{n}_{CH_4;in;REF} &= 0,03971 \text{ [mol/s]} \\
\dot{n}_{CO_2;eq;REF} &= 0,0008753 \text{ [mol/s]} \\
\dot{n}_{CO_2;eq;SOFC} &= 0,0008087 \text{ [mol/s]} \\
\dot{n}_{CO_2;in;SOFC} &= 0,0008753 \text{ [mol/s]} \\
\dot{n}_{CO;eq;REG} &= 0,0004815 \text{ [mol/s]} \\
\dot{n}_{CO;in;SOFC} &= 0,0006284 \text{ [mol/s]} \\
\dot{n}_{gas;out;REG} &= 0,095 \text{ [mol/s]} \\
\dot{n}_{H_2O;eq;REG} &= 0,05541 \text{ [mol/s]} \\
\dot{n}_{H_2O;in;REF} &= 0,1588 \text{ [mol/s]} \\
\dot{n}_{H_2O;in;SOFC} &= 0,08189 \text{ [mol/s]} \\
\dot{n}_{H_2;eq;REF} &= 0,1545 \text{ [mol/s]} \\
\dot{n}_{H_2;eq;SOFC} &= 0,1572 \text{ [mol/s]} \\
\dot{n}_{H_2;in;SOFC} &= 0,1545 \text{ [mol/s]} \\
\dot{n}_{N_2;SOFC} &= 1,509 \text{ [mol/s]} \\
\dot{n}_{O_2;SOFC} &= 0,3773 \text{ [mol/s]} \\
\dot{n}_{tot;eq;REF} &= 0,2388 \text{ [mol/s]} \\
\dot{n}_{tot;in;REF} &= 0,2002 \text{ [mol/s]} \\
\dot{n}_{tot;SOFC} &= 0,2407 \text{ [mol/s]} \\
O_{2Air;comp} &= 0,2 \\
P &= 1 \text{ [atm]} \\
PowerOfMethane &= 33,13 \text{ [kW]} \\
P_0 &= 101,3 \text{ [kPa]} \\
P_{H_2O} &= 0,3367 \\
P_{SOFC} &= 12,1 \text{ [kW]} \\
\dot{Q}_{air;SOFC;in;Burner} &= 45,99 \text{ [kW]} \\
\dot{Q}_{CaO;in;REF} &= 5,608 \text{ [kW]} \\
\dot{Q}_{Catalyst;in;REF} &= 3,798 \text{ [kW]} \\
\dot{Q}_{CH_4;burner;in} &= 15,75 \text{ [kW]}
\end{aligned}$$

$$\begin{aligned}
\dot{Q}_{CH_4,in;REF} &= 0,2813 \text{ [kW]} \\
\dot{Q}_{CH_4,out;REF} &= 0,02735 \text{ [kW]} \\
\dot{Q}_{CO_2,in;REF} &= 0,01215 \text{ [kW]} \\
\dot{Q}_{CO_2,out;REF} &= 0,02366 \text{ [kW]} \\
\dot{Q}_{CO,in;SOFC} &= 0,01293 \text{ [kW]} \\
\dot{Q}_{CO,out;SOFC} &= 0,0379 \text{ [kW]} \\
\dot{Q}_{H_2O,in;SOFC} &= 2,139 \text{ [kW]} \\
\dot{Q}_{H_2O,out;SOFC} &= 4,738 \text{ [kW]} \\
\dot{Q}_{H_2,out;REF} &= 2,605 \text{ [kW]} \\
\dot{Q}_{H_2,rxn;SOFC} &= -18,26 \text{ [kJ/s]} \\
\dot{Q}_{HeatExchanger,out} &= 48,65 \text{ [kW]} \\
\dot{Q}_{in;CaO;REG} &= 2,419 \text{ [kW]} \\
\dot{Q}_{in;H_2O;REG} &= 1,48 \text{ [kW]} \\
\dot{Q}_{in;MgO;REG} &= 2,637 \text{ [kW]} \\
\dot{Q}_{loss;REG} &= 0 \text{ [kW]} \\
\dot{Q}_{MgO,in;REF} &= 4,291 \text{ [kW]} \\
\dot{Q}_{N_2,in;cat;SOFC} &= 33,42 \text{ [kW]} \\
\dot{Q}_{O_2,in;cat;SOFC} &= 8,922 \text{ [kW]} \\
\dot{Q}_{out;CaO;REG} &= 5,608 \text{ [kW]} \\
\dot{Q}_{out;CO_2;REG} &= 1,585 \text{ [kW]} \\
\dot{Q}_{out;H_2;REG} &= 0,01529 \text{ [kW]} \\
\dot{Q}_{rxn;Carb;REF} &= -6,233 \text{ [kW]} \\
\dot{Q}_{rxn;WGS;REF} &= -1,565 \text{ [kW]} \\
\dot{Q}_{solids,out;REF} &= 10,44 \text{ [kW]} \\
\dot{Q}_{WGS;rxn;SOFC} &= 0,002731 \text{ [kW]} \\
r_{Cell} &= 0,348 \text{ [\Omega \cdot cm}^2\text{]} \\
T_{otBioGas} &= 0,0418 \text{ [mol/s]} \\
T_{calc} &= 1123 \text{ [K]} \\
\boxed{T_{in;cat;SOFC} = 1024 \text{ [K]}} \\
\boxed{T_{in;REF} = 475,5 \text{ [K]}} \\
T_{in;SOFC} &= 1003 \text{ [K]} \\
T_{out;burner} &= 1323 \text{ [K]} \\
T_{out;REF} &= 873,2 \text{ [K]} \\
T_{SOFC} &= 1103 \text{ [K]} \\
V_{nernst} &= 0,9758 \text{ [V]} \\
x_1 &= 0,03879 \text{ [mol/s]} \\
x_2 &= 0,03816 \text{ [mol/s]} \\
x_3 &= 0,03896 \text{ [mol/s]} \\
x_{reg} &= 0,03896 \text{ [mol/s]} \\
Y_{CH_4,out;dry;SOFC} &= 0,00004852 \\
Y_{CO_2,out;dry;SOFC} &= 0,009607 \\
Y_{CO,dry;REF} &= 0,004004 \\
Y_{CO,out;REG} &= 0,005069 \\
Y_{H_2,dry;REF} &= 0,9846 \\
Y_{H_2,out;REG} &= 0,0066
\end{aligned}$$

$$\begin{aligned}
\dot{Q}_{CH_4,in;SOFC} &= 0,03599 \text{ [kW]} \\
\dot{Q}_{CH_4,out;SOFC} &= 0,0001915 \text{ [kW]} \\
\dot{Q}_{CO_2,in;SOFC} &= 0,02995 \text{ [kW]} \\
\dot{Q}_{CO_2,out;SOFC} &= 0,03229 \text{ [kW]} \\
\dot{Q}_{CO,out;REF} &= 0,01053 \text{ [kW]} \\
\dot{Q}_{H_2O,in;REF} &= 1,024 \text{ [kW]} \\
\dot{Q}_{H_2O,out;REF} &= 1,713 \text{ [kW]} \\
\dot{Q}_{H_2,in;SOFC} &= 3,202 \text{ [kW]} \\
\dot{Q}_{H_2,out;SOFC} &= 1,939 \text{ [kW]} \\
\dot{Q}_{HeatExchanger,in} &= 60,96 \text{ [kW]} \\
\dot{Q}_{in;CaCO_3;REG} &= 2,145 \text{ [kW]} \\
\dot{Q}_{in;Catalyst;REG} &= 2,241 \text{ [kW]} \\
\dot{Q}_{in;H_2;REG} &= 0,02363 \text{ [kW]} \\
\dot{Q}_{loss;REF} &= 0 \text{ [kW]} \\
\dot{Q}_{loss;SOFC} &= 0,6052 \text{ [kW]} \\
\dot{Q}_{MgO,out;REF} &= 2,916 \text{ [kW]} \\
\dot{Q}_{N_2,out;SOFC} &= 37,38 \text{ [kW]} \\
\dot{Q}_{O_2,out;SOFC} &= 8,992 \text{ [kW]} \\
\dot{Q}_{out;Catalyst;REG} &= 3,798 \text{ [kW]} \\
\dot{Q}_{out;H_2O;REG} &= 1,729 \text{ [kW]} \\
\dot{Q}_{out;MgO;REG} &= 4,291 \text{ [kW]} \\
\dot{Q}_{rxn;SR;REF} &= 7,991 \text{ [kW]} \\
\dot{Q}_{solids,in;REF} &= 13,7 \text{ [kW]} \\
\dot{Q}_{SR;rxn;SOFC} &= 0,1888 \text{ [kW]} \\
Ratio_{CaO;CH_4} &= 3,27 \\
SteamCarbonRatio &= 4 \\
T_0 &= 298,2 \text{ [K]} \\
T_{in;burner} &= 1073 \text{ [K]} \\
T_{in;HeatExchanger} &= 1323 \text{ [K]} \\
T_{in;REG} &= 1023 \text{ [K]} \\
T_{in;solids;REG} &= 818,2 \text{ [K]} \\
T_{out;HeatExchanger} &= 1133 \text{ [K]} \\
T_{out;REG} &= 1125 \text{ [K]} \\
V_{FC;Cell} &= 0,8749 \text{ [V]} \\
V_{tot} &= 0,1009 \text{ [V]} \\
x_{1;sofc} &= 0,0009166 \text{ [mol/s]} \\
x_{2;sofc} &= -0,00006661 \text{ [mol/s]} \\
x_4 &= 0,0004815 \text{ [mol/s]} \\
Y_{CH_4,dry;REF} &= 0,005866 \\
Y_{CO_2,dry;REF} &= 0,005577 \\
Y_{CO_2,out;REG} &= 0,405 \\
Y_{CO,out;dry;SOFC} &= 0,01915 \\
Y_{H_2O,out;REG} &= 0,5833 \\
Y_{H_2,out;dry;SOFC} &= 0,9712
\end{aligned}$$



# Appendix D

## Solution made in EES for the ZEG400

$AirFlowCathode = 1,041$  [kg/s]  
 $CH4 = 0,95$   
 $Comp_{H2O;in;REG} = 0,9802$   
 $C_{p;air;burner;in} = 1,071$  [kJ/kg-K]  
 $C_{p;air;burner;SOFC;in} = 1,075$  [kJ/kg-K]  
 $C_{p;air;HeatExchanger;out} = 1,079$  [kJ/kg-K]  
 $C_{p;CaO;in;REF} = 0,9312$  [kJ/K-kg]  
 $C_{p;CaO;out;REF} = 0,9128$  [kJ/K-kg]  
 $C_{p;Catalyst;in;REF} = 1,072$  [kJ/kg-K]  
 $C_{p;CH4;in;REF} = 2,489$  [kJ/kg-K]  
 $C_{p;CH4;SOFC} = 3,456$  [kJ/kg-K]  
 $C_{p;CO2;in;REF} = 0,9309$  [kJ/kg-K]  
 $C_{p;CO2;out;REG} = 1,132$  [kJ/kg-K]  
 $C_{p;CO2;SOFC;out} = 1,127$  [kJ/kg-K]  
 $C_{p;CO;SOFC} = 1,042$  [kJ/kg-K]  
 $C_{p;H2O;in;REF} = 2,016$  [kJ/kg-K]  
 $C_{p;H2O;out;REF} = 2,02$  [kJ/kg-K]  
 $C_{p;H2O;SOFC} = 2,057$  [kJ/kg-K]  
 $C_{p;H2;in;REG} = 14,58$  [kJ/kg-K]  
 $C_{p;H2;out;REG} = 14,62$  [kJ/kg-K]  
 $C_{p;H2;SOFC;out} = 14,61$  [kJ/kg-K]  
 $C_{p;MgO;out;REF} = 1,076$  [kJ/kg-K]  
 $C_{p;N2;SOFC;out} = 1,098$  [kJ/kg-K]  
 $C_{p;O2;SOFC;out} = 1,028$  [kJ/kg-K]  
 $C_{p;850;CaO} = 51,19$  [kJ/kmol-K]  
 $\Delta H_{rxn;Carb} = -160$  [kJ/mol]  
 $\Delta H_{rxn;WGS} = -41$  [kJ/mol]  
 $\delta \dot{Q}_{in;REF} = 25,23$  [kW]  
 $\Delta \dot{Q}_{in;SOFC} = 914,9$  [kW]  
 $\delta \dot{Q}_{out;REF} = 83,9$  [kW]  
 $\Delta \dot{Q}_{out;SOFC} = 1017$  [kW]  
 $\delta \dot{Q}_{rxn;REF} = 3,693$  [kW]  
 $\Delta \dot{Q}_{rxn;SOFC} = -346$  [kW]  
 $\Delta Q_{out;REG} = 445,6$  [kW]  
 $\eta_{CoGeneration} = 0,65$   
 $E^0 = 0,9826$  [V]  
 $FU = 0,48$   
 $HeatLoss = 0,05$   
 $I_{Cell} = 36,83$  [A]  
 $J_{FC;Cell} = 0,29$  [A/cm<sup>2</sup>]  
 $K_{p;SR} = 0,5391$  [atm<sup>2</sup>]  
 $K_{p;WGS} = 2,628$   
 $K_{p;WGS;SOFC} = 0,9734$   
 $LHV_{CO} = 10000$  [kJ/kg]  
 $loss = 0$   
 $\dot{m}_{air;burner;in} = 0,01101$  [kg/s]  
 $\dot{m}_{air;SOFC;in;Burner} = 1,018$  [kg/s]  
 $\dot{m}_{CaCO3;out;REF} = 0,07469$  [kg/s]  
 $\dot{m}_{CaO;in;REG} = 0,09764$  [kg/s]  
 $\dot{m}_{CaO;out;REG} = 0,1395$  [kg/s]  
 $\dot{m}_{Catalyst;in;REG} = 0,08206$  [kg/s]

$CaO_{per;CD} = 0,618$   
 $CO2 = 0,04$   
 $Comp_{H2;in;REG} = 0,01978$   
 $C_{p;air;burner;out} = 1,101$  [kJ/kg-K]  
 $C_{p;air;HeatExchanger;in} = 1,101$  [kJ/kg-K]  
 $C_{p;CaCO3;REF} = 1,058$  [kJ/kg-K]  
 $C_{p;CaO;in;REG} = 0,9128$  [kJ/K-kg]  
 $C_{p;CaO;out;REG} = 0,9312$  [kJ/K-kg]  
 $C_{p;Catalyst;out;REF} = 1,006$  [kJ/kg-K]  
 $C_{p;CH4;out;REF} = 3,22$  [kJ/kg-K]  
 $C_{p;CH4;SOFC;out} = 3,631$  [kJ/kg-K]  
 $C_{p;CO2;out;REF} = 1,068$  [kJ/kg-K]  
 $C_{p;CO2;SOFC} = 1,103$  [kJ/kg-K]  
 $C_{p;CO;out;REF} = 1,041$  [kJ/kg-K]  
 $C_{p;CO;SOFC;out} = 1,043$  [kJ/kg-K]  
 $C_{p;H2O;in;REG} = 2,063$  [kJ/kg-K]  
 $C_{p;H2O;out;REG} = 2,094$  [kJ/kg-K]  
 $C_{p;H2O;SOFC;out} = 2,087$  [kJ/kg-K]  
 $C_{p;H2;out;REF} = 14,54$  [kJ/kg-K]  
 $C_{p;H2;SOFC} = 14,58$  [kJ/kg-K]  
 $C_{p;MgO;in;REF} = 1,101$  [kJ/kg-K]  
 $C_{p;N2;SOFC} = 1,089$  [kJ/kg-K]  
 $C_{p;O2;SOFC} = 1,018$  [kJ/kg-K]  
 $C_{p;850} = 52,22$  [kJ/kmol-K]  
 $\Delta H_{rxn;Calc} = 160$  [kJ/mol]  
 $\Delta H_{rxn;SR} = 206$  [kJ/mol]

$\Delta \dot{Q}_{HEAT;NEED;REG} = 235,9$  [kW]

$\delta \dot{Q}_{in;REG} = 28,8$  [kW]  
 $\delta \dot{Q}_{in;solids;REG} = 180,9$  [kW]  
 $\delta \dot{Q}_{out;REG} = 63,79$  [kW]  
 $\delta \dot{Q}_{out;solids;REG} = 262,4$  [kW]  
 $\delta \dot{Q}_{rxn;REG} = 119,4$  [kW]  
 $\Delta Q_{in;REG} = 445,6$  [kW]  
 $\eta_{burner} = 0,98$   
 $\eta_{StandAlone} = 0,76$   
 $Faraday = 96487$  [Coulomb/mol]  
 $HeatGenerated = 117,9$  [kW]  
 $HydrogenPowerREF = 716,1$  [kW]  
 $I_{FC} = 278945$  [A]  
 $K_{p;CO2} = 2,693$  [1/kPa]  
 $K_{p;SR;SOFC} = 326,6$  [atm<sup>2</sup>]  
 $K_{p;WGS;REG} = 1,106$   
 $LHV_{CH4} = 52000$  [kJ/kg]  
 $LHV_{H2} = 120000$  [kJ/kg]  
 $Loss_{REG} = 0$   
 $\dot{m}_{air;burner;out} = 1,035$  [kg/s]  
 $\dot{m}_{CaCO3;in;REG} = 0,07469$  [kg/s]  
 $\dot{m}_{CaO;in;REF} = 0,1395$  [kg/s]  
 $\dot{m}_{CaO;out;REF} = 0,09764$  [kg/s]  
 $\dot{m}_{Catalyst;in;REF} = 0,08206$  [kg/s]  
 $\dot{m}_{Catalyst;out;REF} = 0,08206$  [kg/s]

$\dot{m}_{CH_4;burner;in} = 0,0058$  [kg/s]  
 $\dot{m}_{CH_4;in;SOFC} = 0,0002829$  [kg/s]  
 $\dot{m}_{CH_4;SOFC} = 0,000001255$  [kg/s]  
 $\dot{m}_{CO_2;in;SOFC} = 0,0007379$  [kg/s]  
 $\dot{m}_{CO_2;out;REG} = 0,03244$  [kg/s]  
 $\dot{m}_{CO;in;SOFC} = 0,0003372$  [kg/s]  
 $\dot{m}_{CO;SOFC} = 0,0008647$  [kg/s]  
 $\dot{m}_{H_2O;in;REG} = 0,01896$  [kg/s]  
 $\dot{m}_{H_2O;out;REF} = 0,02826$  [kg/s]  
 $\dot{m}_{H_2O;SOFC} = 0,05401$  [kg/s]  
 $\dot{m}_{H_2;in;SOFC} = 0,005968$  [kg/s]  
 $\dot{m}_{H_2;out;REG} = 0,00002421$  [kg/s]  
 $\dot{m}_{H_2;SOFC} = 0,006071$  [kg/s]  
 $\dot{m}_{HeatExchanger;out} = 1,035$  [kg/s]  
 $\dot{m}_{in;SOFC} = 1,077$  [kg/s]  
 $\dot{m}_{MgO;in;REF} = 0,09028$  [kg/s]  
 $\dot{m}_{MgO;out;REF} = 0,09028$  [kg/s]  
 $\dot{m}_{O_2;in;SOFC} = 0,2313$  [kg/s]  
 $\dot{m}_{out;REF} = 0,03559$  [kg/s]  
 $\dot{m}_{out;solids} = 0,3447$  [kg/s]  
 $\dot{m}_{solids;out;REF} = 0,3447$  [kg/s]  
 $\dot{n}_{CaCO_3;eq;REF} = 0,7463$  [mol/s]  
 $\dot{n}_{CaCO_3;out;REF} = 0,7463$  [mol/s]  
 $\dot{n}_{CaO;eq;REG} = 2,487$  [mol/s]  
 $\dot{n}_{cat;tot;in} = 36,14$  [mol/s]  
 $\dot{n}_{CH_4;eq;SOFC} = 0,00007824$  [mol/s]  
 $\dot{n}_{CH_4;in;SOFC} = 0,01764$  [mol/s]  
 $\dot{n}_{CO_2;eq;REG} = 0,737$  [mol/s]  
 $\dot{n}_{CO_2;in;REF} = 0,03203$  [mol/s]  
 $\dot{n}_{CO;eq;REF} = 0,01204$  [mol/s]  
 $\dot{n}_{CO;eq;SOFC} = 0,03087$  [mol/s]  
 $\dot{n}_{gas;in;REG} = 1,073$  [mol/s]  
 $\dot{n}_{H_2O;eq;REF} = 1,569$  [mol/s]  
 $\dot{n}_{H_2O;eq;SOFC} = 1,552$  [mol/s]  
 $\dot{n}_{H_2O;in;REG} = 1,052$  [mol/s]  
 $\dot{n}_{H_2O;rxn;SOFC} = 1,446$  [mol/s]  
 $\dot{n}_{H_2;eq;REG} = 0,01201$  [mol/s]  
 $\dot{n}_{H_2;in;REG} = 0,02123$  [mol/s]  
 $\dot{n}_{H_2;out;SOFC} = 1,566$  [mol/s]  
 $\dot{n}_{O_2;rxn;SOFC} = 0,7228$  [mol/s]  
 $\dot{n}_{tot;dry;REF} = 3,007$  [mol/s]  
 $\dot{n}_{tot;eq;REG} = 1,82$  [mol/s]  
 $\dot{n}_{tot;out;SOFC} = 1,612$  [mol/s]  
 $n_{total;cells} = 7574$   
 $OU = 0,1$   
 $PowerOfHydrogen = 378,8$  [kW]  
 $PowerOfMethane_{burner} = 301,6$  [kW]  
 $P_{H_2} = 0,6532$   
 $P_{O_2} = 0,2$   
 $\dot{Q}_{air;burner;in} = 9,141$  [kW]  
 $\dot{Q}_{CaCO_3;out;REF} = 45,44$  [kW]  
 $\dot{Q}_{CaO;out;REF} = 51,25$  [kW]  
 $\dot{Q}_{Catalyst;out;REF} = 47,47$  [kW]

$\dot{m}_{CH_4;in;REF} = 0,0122$  [kg/s]  
 $\dot{m}_{CH_4;out;REF} = 0,0002829$  [kg/s]  
 $\dot{m}_{CO_2;in;REF} = 0,00141$  [kg/s]  
 $\dot{m}_{CO_2;out;REF} = 0,0007379$  [kg/s]  
 $\dot{m}_{CO_2;SOFC} = 0,0006817$  [kg/s]  
 $\dot{m}_{CO;out;REF} = 0,0003372$  [kg/s]  
 $\dot{m}_{H_2O;in;REF} = 0,05482$  [kg/s]  
 $\dot{m}_{H_2O;in;SOFC} = 0,02826$  [kg/s]  
 $\dot{m}_{H_2O;out;REG} = 0,01912$  [kg/s]  
 $\dot{m}_{H_2;in;REG} = 0,00004281$  [kg/s]  
 $\dot{m}_{H_2;out;REF} = 0,005968$  [kg/s]  
 $\dot{m}_{H_2;out;SOFC} = 0,003157$  [kg/s]  
 $\dot{m}_{HeatExchanger;in} = 1,035$  [kg/s]  
 $\dot{m}_{in;REF} = 0,06843$  [kg/s]  
 $\dot{m}_{in;solids;REF} = 0,3118$  [kg/s]  
 $\dot{m}_{MgO;in;REG} = 0,09028$  [kg/s]  
 $\dot{m}_{N_2;in;SOFC} = 0,8099$  [kg/s]  
 $\dot{m}_{O_2;out;SOFC} = 0,2081$  [kg/s]  
 $\dot{m}_{out;SOFC} = 1,077$  [kg/s]  
 $\dot{m}_{solids;in;REF} = 0,3118$  [kg/s]  
 $N_{2Air;comp} = 0,8$   
 $\dot{n}_{CaCO_3;eq;REG} = 0$  [mol/s]  
 $\dot{n}_{CaO;eq;REF} = 1,741$  [mol/s]  
 $\dot{n}_{CaO;in;REF} = 2,487$  [mol/s]  
 $\dot{n}_{CH_4;eq;REF} = 0,01764$  [mol/s]  
 $\dot{n}_{CH_4;in;REF} = 0,7607$  [mol/s]  
 $\dot{n}_{CO_2;eq;REF} = 0,01677$  [mol/s]  
 $\dot{n}_{CO_2;eq;SOFC} = 0,01549$  [mol/s]  
 $\dot{n}_{CO_2;in;SOFC} = 0,01677$  [mol/s]  
 $\dot{n}_{CO;eq;REG} = 0,009223$  [mol/s]  
 $\dot{n}_{CO;in;SOFC} = 0,01204$  [mol/s]  
 $\dot{n}_{gas;out;REG} = 1,82$  [mol/s]  
 $\dot{n}_{H_2O;eq;REG} = 1,061$  [mol/s]  
 $\dot{n}_{H_2O;in;REF} = 3,043$  [mol/s]  
 $\dot{n}_{H_2O;in;SOFC} = 1,569$  [mol/s]  
 $\dot{n}_{H_2;eq;REF} = 2,96$  [mol/s]  
 $\dot{n}_{H_2;eq;SOFC} = 3,011$  [mol/s]  
 $\dot{n}_{H_2;in;SOFC} = 2,96$  [mol/s]  
 $\dot{n}_{N_2;SOFC} = 28,91$  [mol/s]  
 $\dot{n}_{O_2;SOFC} = 7,228$  [mol/s]  
 $\dot{n}_{tot;eq;REF} = 4,575$  [mol/s]  
 $\dot{n}_{tot;in;REF} = 3,835$  [mol/s]  
 $\dot{n}_{tot;SOFC} = 4,61$  [mol/s]  
 $O_{2Air;comp} = 0,2$   
 $P = 1$  [atm]  
 $PowerOfMethane = 634,6$  [kW]  
 $P_0 = 101,3$  [kPa]  
 $P_{H_2O} = 0,3367$   

$P_{SOFC} = 231,8$  [kW]

  
 $\dot{Q}_{air;SOFC;in;Burner} = 880,9$  [kW]  
 $\dot{Q}_{CaO;in;REF} = 107,4$  [kW]  
 $\dot{Q}_{Catalyst;in;REF} = 72,75$  [kW]  
 $\dot{Q}_{CH_4;burner;in} = 301,6$  [kW]

$$\begin{aligned}
\dot{Q}_{CH_4,in;REF} &= 5,388 \text{ [kW]} \\
\dot{Q}_{CH_4,out;REF} &= 0,5239 \text{ [kW]} \\
\dot{Q}_{CO_2,in;REF} &= 0,2328 \text{ [kW]} \\
\dot{Q}_{CO_2,out;REF} &= 0,4532 \text{ [kW]} \\
\dot{Q}_{CO,in;SOFC} &= 0,2476 \text{ [kW]} \\
\dot{Q}_{CO,out;SOFC} &= 0,7259 \text{ [kW]} \\
\dot{Q}_{H_2O,in;SOFC} &= 40,97 \text{ [kW]} \\
\dot{Q}_{H_2O,out;SOFC} &= 90,75 \text{ [kW]} \\
\dot{Q}_{H_2,out;REF} &= 49,9 \text{ [kW]} \\
\dot{Q}_{H_2;rxn;SOFC} &= -349,7 \text{ [kJ/s]} \\
\dot{Q}_{HeatExchanger;out} &= 931,9 \text{ [kW]} \\
\dot{Q}_{in;CaO;REG} &= 46,35 \text{ [kW]} \\
\dot{Q}_{in;H_2O;REG} &= 28,35 \text{ [kW]} \\
\dot{Q}_{in;MgO;REG} &= 50,51 \text{ [kW]} \\
\dot{Q}_{loss;REG} &= 0 \text{ [kW]} \\
\dot{Q}_{MgO,in;REF} &= 82,2 \text{ [kW]} \\
\dot{Q}_{N_2,in;cat;SOFC} &= 640,2 \text{ [kW]} \\
\dot{Q}_{O_2,in;cat;SOFC} &= 170,9 \text{ [kW]} \\
\dot{Q}_{out;CaO;REG} &= 107,4 \text{ [kW]} \\
\dot{Q}_{out;CO_2;REG} &= 30,37 \text{ [kW]} \\
\dot{Q}_{out;H_2;REG} &= 0,2928 \text{ [kW]} \\
\dot{Q}_{rxn;Carb;REF} &= -119,4 \text{ [kW]} \\
\dot{Q}_{rxn;WGS;REF} &= -29,97 \text{ [kW]} \\
\dot{Q}_{solids;out;REF} &= 200 \text{ [kW]} \\
\dot{Q}_{WGS;rxn;SOFC} &= 0,05231 \text{ [kW]} \\
r_{Cell} &= 0,348 \text{ [\Omega \cdot cm}^2\text{]} \\
T_{otBioGas} &= 0,8007 \text{ [mol/s]} \\
T_{calc} &= 1123 \text{ [K]} \\
\boxed{T_{in;cat;SOFC} = 1024 \text{ [K]}} \\
\boxed{T_{in;REF} = 475,5 \text{ [K]}} \\
T_{in;SOFC} &= 1003 \text{ [K]} \\
T_{out;burner} &= 1323 \text{ [K]} \\
T_{out;REF} &= 873,2 \text{ [K]} \\
T_{SOFC} &= 1103 \text{ [K]} \\
V_{nernst} &= 0,9758 \text{ [V]} \\
x_1 &= 0,743 \text{ [mol/s]} \\
x_2 &= 0,731 \text{ [mol/s]} \\
x_3 &= 0,7463 \text{ [mol/s]} \\
x_{reg} &= 0,7463 \text{ [mol/s]} \\
Y_{CH_4;out;dry;SOFC} &= 0,00004852 \\
Y_{CO_2;out;dry;SOFC} &= 0,009607 \\
Y_{CO;dry;REF} &= 0,004004 \\
Y_{CO;out;REG} &= 0,005069 \\
Y_{H_2;dry;REF} &= 0,9846 \\
Y_{H_2;out;REG} &= 0,0066
\end{aligned}$$

$$\begin{aligned}
\dot{Q}_{CH_4,in;SOFC} &= 0,6894 \text{ [kW]} \\
\dot{Q}_{CH_4,out;SOFC} &= 0,003669 \text{ [kW]} \\
\dot{Q}_{CO_2,in;SOFC} &= 0,5738 \text{ [kW]} \\
\dot{Q}_{CO_2,out;SOFC} &= 0,6186 \text{ [kW]} \\
\dot{Q}_{CO,out;REF} &= 0,2017 \text{ [kW]} \\
\dot{Q}_{H_2O,in;REF} &= 19,61 \text{ [kW]} \\
\dot{Q}_{H_2O,out;REF} &= 32,82 \text{ [kW]} \\
\dot{Q}_{H_2,in;SOFC} &= 61,33 \text{ [kW]} \\
\dot{Q}_{H_2,out;SOFC} &= 37,14 \text{ [kW]} \\
\dot{Q}_{HeatExchanger;in} &= 1168 \text{ [kW]} \\
\dot{Q}_{in;CaCO_3;REG} &= 41,09 \text{ [kW]} \\
\dot{Q}_{in;Catalyst;REG} &= 42,93 \text{ [kW]} \\
\dot{Q}_{in;H_2;REG} &= 0,4526 \text{ [kW]} \\
\dot{Q}_{loss;REF} &= 0 \text{ [kW]} \\
\dot{Q}_{loss;SOFC} &= 11,59 \text{ [kW]} \\
\dot{Q}_{MgO,out;REF} &= 55,86 \text{ [kW]} \\
\dot{Q}_{N_2,out;SOFC} &= 716 \text{ [kW]} \\
\dot{Q}_{O_2,out;SOFC} &= 172,3 \text{ [kW]} \\
\dot{Q}_{out;Catalyst;REG} &= 72,75 \text{ [kW]} \\
\dot{Q}_{out;H_2O;REG} &= 33,12 \text{ [kW]} \\
\dot{Q}_{out;MgO;REG} &= 82,2 \text{ [kW]} \\
\dot{Q}_{rxn;SR;REF} &= 153,1 \text{ [kW]} \\
\dot{Q}_{solids;in;REF} &= 262,4 \text{ [kW]} \\
\dot{Q}_{SR;rxn;SOFC} &= 3,617 \text{ [kW]} \\
Ratio_{CaO;CH_4} &= 3,27 \\
SteamCarbonRatio &= 4 \\
T_0 &= 298,2 \text{ [K]} \\
T_{in;burner} &= 1073 \text{ [K]} \\
T_{in;HeatExchanger} &= 1323 \text{ [K]} \\
T_{in;REG} &= 1023 \text{ [K]} \\
T_{in;solids;REG} &= 818,2 \text{ [K]} \\
T_{out;HeatExchanger} &= 1133 \text{ [K]} \\
T_{out;REG} &= 1125 \text{ [K]} \\
V_{FC;Cell} &= 0,8749 \text{ [V]} \\
V_{tot} &= 0,1009 \text{ [V]} \\
x_{1;sofc} &= 0,01756 \text{ [mol/s]} \\
x_{2;sofc} &= -0,001276 \text{ [mol/s]} \\
x_4 &= 0,009223 \text{ [mol/s]} \\
Y_{CH_4;dry;REF} &= 0,005866 \\
Y_{CO_2;dry;REF} &= 0,005577 \\
Y_{CO_2;out;REG} &= 0,405 \\
Y_{CO;out;dry;SOFC} &= 0,01915 \\
Y_{H_2O;out;REG} &= 0,5833 \\
Y_{H_2;out;dry;SOFC} &= 0,9712
\end{aligned}$$





Norges miljø- og biovitenskapelig universitet  
Noregs miljø- og biovitenskapelige universitet  
Norwegian University of Life Sciences

Postboks 5003  
NO-1432 Ås  
Norway