Modelling of Tandem SOFC and PEMFC Fuel Cell Systems for Maritime Application

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TU Delft

Modelling of Tandem SOFC and PEMFC Fuel Cell Systems for Maritime Application

By

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TU Delft

Preface

This report presents the whole process of the study of S. Zhao's master thesis. The abstract can be found in the very beginning of the main text. The study of this master thesis is the first stage of the project on applying tandem fuel cell systems in marine industry. The layout of the whole project and the task of this thesis are stated in **Chapter 1**. Although the concept of a tandem SOFC and PEMFC system has been existing long, this project is the very first one that is concerned to marine application. The final goal of this project is to apply a real tandem fuel cell system on a ship. However, it may take a long time before this can be realized. But with a solid foundation, the further development would be smoother. This is exactly what this master thesis is meant to provide.

When looking back at this whole year, I am glad to say that I have not only acquired ample knowledge on fuel cell systems, system modelling and doing scientific research, but also learnt how to be the project manager of myself. Working alone may be difficult and tedious sometimes, but it provides me with a great chance of training my ability of solving problems alone and seeking for help from available resources.

I would like to give special thanks to my supervisor Ir. P. de Vos, who always gave me effective and timely guidance on my study whenever I was in the wrong direction. When I made a mistake, even for the smallest ones, he would patiently help me fix them. I am also grateful to Ir. L. van Biert who gave me plenty of help on understanding the technical details of fuel cells. As a marine engineering student, fuel cell systems were totally a new field for me when I started. But with their help, I was able to familiarize with fuel cells quickly and perform my study smoothly. Last but not the least, I really appreciate it that my chairman Ir. K. Visser gave me this intriguing topic, in which I have developed real enthusiasm after the whole-year study.

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Nomenclature

A_{FC}	active cell area (m^2)
C_P	specific heat (J/kgK)
E	open circuit voltage of the fuel cell (V)
E_{fuel}	total chemical energy contained in the fuel (KW)
F	Faraday's constant (C/mole);
h	specific enthalpy (KJ/kgs)
i	current density (A/m^2)
I	current (A)
$K_{reaction}$	equilibrium constant (-)
$\dot{m}$	mass flow (kg/s)
m	mass (kg)
P	pressure (bar)
P	power (KW)
Q	heat (KW)
R	specific gas constant (KJ/moleK)
t	time (s)
T	temperature (K)
V	Voltage (V)
x	reaction coordinate of the reaction (-)
x_i	mass fraction of components (-)
y_i	mole fraction of components (-)
μ_{fuel}	fuel utilization factor (-)
Φ	mass flow (kg/s)
η	efficiency (-)

Abstract

The world is moving towards a cleaner future. With the increasingly stringent emission regulation in maritime field and the limitation of marine diesel engine systems, the ship builders may start to seek cleaner solutions rather than modifying the currently prevailing internal combustion engine systems (ICE). According to previous researches, a tandem fuel cell system power plant, which uses LNG as fuel, has a very good overall emission performance in comparison to marine LNG based ICE systems, and can achieve an overall efficiency of more than 60%. To study whether the tandem fuel cell system can be an alternative for marine LNG engine systems, two models are built in this master thesis to study the performance of the system under stationary operation and transients. The first model is built to study the stationary performance of the system, and to verify the result of high efficiency from previous researches. The result shows that indeed an efficiency of almost 60% can be reproduced. The second model is built to study the transient behaviour of the system, and to compare it with that of marine LNG engine systems. The result shows that the system has a better transient response than the recommended transient response for current marine LNG engine systems. Since the SOFC in the tandem fuel cell system has a slow transient behaviour, a hydrogen tank is added between the SOFC system and the PEMFC system as an energy buffer. A design assistance tool is developed to assist in sizing the hydrogen tank and the fuel (LNG) tank in design phase.

1. Introduction

1.1 Background

The world is moving towards a cleaner future. Emission reduction has become one of the priorities among most of the traditional industries. From hybrid power vehicles to electric power trains, from local based solar power systems to large scale offshore windfarms, various solutions for emission reduction has been applied and proved effective. In marine industry, this trend also applies. No mater from the perspective of regulation makers, or from the perspective of the shipbuilders, the race of moving towards “cleaner” is getting increasingly intense. Especially in recent years, with a more and more stringent regulation from IMO (International Maritime Organization), the marine engine builders are experiencing unprecedently pressure in the progress of emission reduction. **Figure 1-1** illustrates how strict the limits on NOx emission and sulfur content in fuels are in emission control areas.

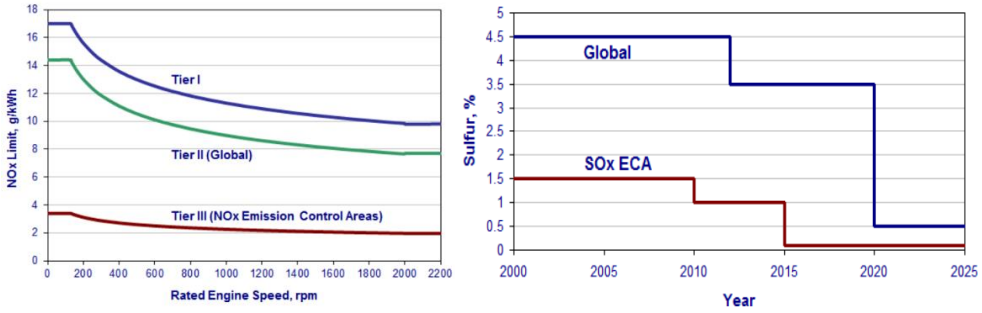


Figure 1-1 IMO regulations on NOx and fuel sulfur content

Currently, in marine industry, the most prevailing onboard electric power generation systems are still the ones based on Internal Combustion Engines (ICE), which are running on Heavy Fuel Oil (HFO), Marine Diesel Oil (MDO), and sometimes Liquified Natural Gas (LNG) nowadays. Among them, HFO is the cheapest, but with a high content of sulfur, which is the origin of SOx emission; MDO is less cheap, but the sulfur content is much lower than that of HFO; LNG, which is gaining more and more popularity recently, has an equivalent price to MDO and an even lower sulfur content (Poten & Partners, 2015). More details of using LNG as marine fuel will be introduced later.

Apart from SOx emission, NOx emission is another main consideration. It should be mention that no matter running on which type of fuel, because of the working principle of ICE (high temperature combustion in cylinders), NOx emission is inevitable for ICE-based onboard electric power generation systems.

Because of the fuel being used and the high temperature combustion feature, those abovementioned ICE-based onboard electric power generation systems can hardly comply with new emission regulations. To keep ICE-based onboard electric power generation systems still operating on the sea, measures are urgently to be taken.

NOx and SOx are two main pollutants being limited in the regulation. Different methods are taken to reduce them. For NOx emission reduction, there have been multiple solutions, among which, the SCR solution turns out to be very effective. SCR is short for Selective Catalytic Reduction. An SCR system is able to convert NOx in the exhaust gas of ICE into nitrogen and water. It is reported that SCR

technology alone can achieve NOx reductions up to 90 percent. (Dieselforum.org) Although the SCR system makes a rather satisfactory solution, the ICE & SCR system contains the following inherent problems:

- Noise: combustion and reciprocate movement create inevitable noise;
- NOx emission: NOx emission can never be completely eliminated;
- System complexity: the SCR system makes the already complex ICE system even more complex.
- High cost

For SOx reduction, the best way is to use cleaner alternative fuels (such as MDO and LNG), since almost all the SOx emission is from the sulfur content in the fuel. Among alternative fuels, LNG has acquired favorable status. The reasons are: (Thorstensen, 2001)

- The sulfur content of natural gas is significantly lower than that of HFO and even lower than MDO
- The energy density of LNG is relatively high among all the alternative fuels, while the cost is equivalent to that of MDO
- Natural gas refilling infrastructure is getting more accessible for ships
- Technology development in LNG storage has made it more reliable and economical
- Depending on the LNG supply method to the cylinders, LNG engines may also have low NOx emission

The ICE that can use LNG as fuel are marine LNG engines. These engines are normally dual fuel engines that burn natural gas or bunker fuel. In emission control areas, natural gas is used as primary fuel; while in other areas, bunker fuel is used. Due to the low content of sulfur in LNG, the SOx emission of this type of engines can be significantly lower than conventional marine ICE running on HFO or even MDO. However, problems still exist for ships using this type of engines.

- Since marine LNG engines are still internal combustion engines, NOx emission still occurs
- Because of the narrow range of air excess ratio, the transient response of marine LNG engines is slower than that of conventional marine diesel engines (Keitaro, Takahisa, Koichi, Tomohiro, & Kazuhiro, 2015)
- Efficiency is comparable to or somewhat lower than conventional marine diesel engines (Gupta, Biruduganti, & Sekar, 2012)

One could argue that a combination of SCR and marine LNG engines can make a better solution in terms of emission reduction, since both SOx and NOx can be significantly reduced. This is true, but the cost and complexity of the system would be brought up to an even higher level in this way, while the drawbacks of LNG engines (such as noise and slow transient response) still exist.

By now, one may ask: are there any better solutions than marine LNG engines & SCR systems that can avoid the inherent drawbacks of internal combustion engines, while maintaining equivalent or better performance? To answer this question, our focus should be moved to power plants without internal combustion engines.

Desirable alternatives to marine LNG-based ICE power plants are not easy to find. There have already been several attempts. However, although most of them can solve the emission and noise problems to a large extent, applying them onboard ships brings more other issues. For example, solar-power

power plant, which is rather clean and silent. But they need a large amount of deck area to generate sufficient electricity. For most ships, the deck area is rather valuable. Using the deck area only for power generating would greatly bring down the economy of the ship. Another possibility is to store electricity by batteries instead of onboard generation. This is also a clean and silent solution, but for the given technology, the power density of batteries is so low that the electric power solely from them is not sufficient for long range sailing. Besides, the charging time of batteries is much longer than refilling fuel tanks. So, is there an option that can solve the emission and noise problems while not bring too much extra problems? The answer is yes, and that option is LNG-based fuel cell system.

Before going into details of natural gas fuel cell systems, it is necessary to have a basic overview of fuel cells. Fuel cells are electrochemical cells that can convert chemical energy from fuel into electricity and heat through electrochemical reaction. Since there is no combustion involved throughout the energy conversion process, most drawbacks of internal combustions engines can be avoided. Compared with Marine LNG engines, fuel cells have the following merits:

- Much lower NOx formation due to the absence of sufficiently high temperature
- Modular in nature, which means power production can be distributed relatively freely, thereby reducing the electricity transport losses;
- Noise and vibrations are significantly lower because of the absence of combustion and reciprocating movement;
- Higher overall efficiency can be achieved.

Due to all these advantages over marine LNG engines, in recent years, more attentions have been drawn to the application of fuel cell systems in marine industry. Extensive study on them have been conducted to see if they can make a potential alternative of ICE-based power generation systems. An overview of the applications of fuel cell systems in marine industry can be found in (Biert, Godjevac, Visser, & Aravind, 2016).

LNG-based fuel cells are fuel cells that can directly consume natural gas as fuel, just like marine LNG engines. An example of such kind of fuel cell is SOFC (Solid Oxide Fuel Cells). For most other fuel cells, LNG is not a viable fuel since the only fuel that they can rely on is pure hydrogen. Compared with natural gas (whose availability has been discussed), the availability of hydrogen is much lower no matter in terms of refilling infrastructure or onboard storage. (FathomShipping, 2013) For those fuel cells, applying them onboard will again bring more issues than benefits, and because of the low availability of hydrogen they can hardly outperform marine LNG engines. But this is not the case for natural gas fuel cells, since in terms of fuel availability, they are equivalent to marine LNG engines.

However, there is a main drawback of natural gas fuel cells: poor transient response. Natural gas fuel cells are mostly high temperature fuel cells (up to 1000 °C). The transient behavior of high temperature fuel cells is much worse than that of Marine LNG engines. (Dario Marra, 2016) The transient response of natural gas fuel cells to load change is so slow that their application is almost only limited to stationary if they are not hybridized with other systems. This feature makes this type of fuel cells impossible to replace marine LNG engines if they are used alone, because the electric power demand onboard ships always experiences plenty of transients. But this is only the case when they are used alone. If a hybrid system can be designed as such that it can fully take advantage of all the merits of fuel cells, while improving the transient behavior of the system to an equivalent level as marine LNG engine power plant, then the system will still have a great potential to be an alternative of marine LNG

engine power plant. With this thought in mind, focus is moved to PEMFCs.

PEMFC is short for Proton Exchange Membrane Fuel Cell. They are another type of fuel cells which have the common merits of fuel cells (low noise, low emission and high efficiency). PEMFCs are also characterized by their relatively fast transient response. Without any limitation, the transient behavior of a PEMFC can reach as fast as batteries. Although manufacturers often put a rate limiter in a PEMFC system to limit the transient response for safety purpose (Andreasen, Kær, Justesen, & Sahlin, 2016), their transient response is still faster than that recommended for marine LNG engines. If they can be hybridized with natural gas fuel cells and cover the transient in a hybrid system, then the hybrid system would be desirable.

However, a main problem of this hybrid system is fuel. Unlike natural gas fuel cells, the most commonly used PEMFCs are running on pure hydrogen. This means that if the natural gas fuel cell and the PEMFC are going to use different fuel sources in the hybrid system, large scale onboard hydrogen storage system should be employed in addition to LNG storage system. To store hydrogen onboard ships, there are mainly two ways: stored in the form of pure hydrogen and stored in the form of compound. In both cases, problems would arise: if energy is stored in the form of pure hydrogen, the required amount will be relatively large. Although hydrogen storage has become safer and more effective than it used to be, the limited amount of refilling infrastructure onshore would have great impact on the sailing area of the ship (they can only sail within the area where there is hydrogen refilling infrastructure). If energy is stored in the form of compounds, onboard conversion system (which can convert the stored compound into pure hydrogen) will be required, which not only brings up the complexity of the whole system, but also consumes extra energy. So, is there any way that large scale onboard hydrogen storage system can be avoided? To answer this question, focus is zoomed into another important eye-catching feature of the high temperature LNG-based fuel cells.

For high temperature LNG-based fuel cells, they are capable of converting methane into hydrogen when generating electricity. At certain operation modes, they can be used as natural gas reformer to generate hydrogen. SOFC is one type of high temperature LNG-based fuel cells, and is going to be studied in this thesis. With this feature, the abovementioned onboard hydrogen storage problems can be solved:

- First, methane is the main components of natural gas, which means the only fuel required for the hybrid system is LNG. The required hydrogen for the PEMFC can be produced from the SOFC;
- Besides, unlike other onboard conversion systems which consumes energy, the onboard converting process of SOFC can generate electricity while converting the natural gas into hydrogen and other by-products. This will bring up the overall efficiency of the system to a higher level.

It should be mentioned that when SOFC converts methane into hydrogen, there is also carbon monoxide being produced. Carbon monoxide is toxic for PEMFC, so it must be removed from the gas mixture. Therefore, a gas processing system is employed between the SOFC system and the PEMFC system to purify the hydrogen to the level that can be used by the PEMFC. The main part of the gas processing system is a double stage water gas shift system in which carbon monoxide reacts with steam producing even more hydrogen and carbon dioxide. After the water gas shift system, a pressure

swing adsorption (PSA) system will be employed to remove the carbon dioxide, and separate hydrogen of high purity. The details of the gas processing system will be explained in **Chapter 2**.

So far, the layout of the hybrid system is clear: A SOFC, a gas processing system, and a PEMFC. In this project, this hybrid system is called the “tandem fuel cell system”.

According to the introduction above, it can be concluded that compared with marine LNG engine power plant, the tandem fuel cell system has the following merits:

- NOx emission can be almost eliminated;
- Noise can be reduced;
- The efficiency of the whole system can potentially be higher;
- The transient response can be equivalent or faster.

The concept of hybrid SOFC and PEMFC system has been existing for years. Relevant research papers can be found in (Andrew L. Dicks, 1999) (Abid Rabbani, 2014) (Fernandes, Woudstra, Wijk, Verhoef, & L. Aravind, 2016) (M. Yokoo, 2006). These studies analyze the system by modeling and simulation. All these works focus on the stationary performance of the system. The most recent one is (Fernandes, Woudstra, Wijk, Verhoef, & L. Aravind, 2016), in which the application of the tandem fuel cell system in automobile industry is analyzed. The result turned out that the overall efficiency of the system can reach 60% in certain operation models. Being ware of the great potential of the system, as a marine engineer, it is intriguing to investigate the possibility of applying this system in marine industry. If similar performance could be achieved in marine industry, this system would be reasonably considered as a potential alternative for marine LNG engine power plant. Above all, it can be said that it is more than worthwhile to start a project of studying the application of tandem fuel cell system in marine industry, and see if they can make a viable alternative to the marine LNG engine power plant.

1.2 Layout of the whole project

Based on the background, the project "Tandem FC in Marine Application" is launched **Figure 1-2** shows all the stages of the project.

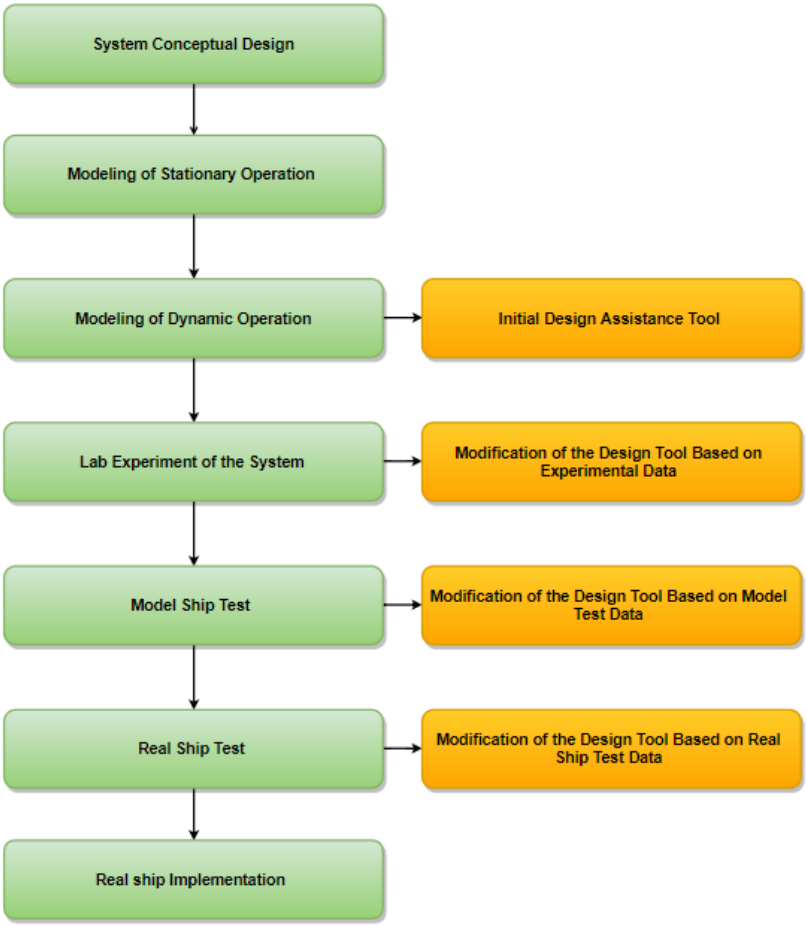


Figure 1-2 Overview of the "Tandem FC in Marine Application" project

As can be seen from **Figure 1-2**, the final goal of this project is to implement the tandem fuel cell system onboard a real ship. Before that, a series of tests through modeling and experiment should be performed. First, a system conceptual design should be proposed as a starting point of the study. Next, model-based design and tests will be done through the modeling of stationary operation and dynamic operation of the system. Once the results from the modeling phase prove the feasibility of the system, the system can be tested through lab experiment to examine its behavior in practice. After that, the system should go through model ship test and real ship test to further analyze the performance of the system when being applied onboard ships.

As can be noticed, throughout the whole project, a design assistance tool is developed and constantly updated as the project moves further. This tool is meant to facilitate the design phase after the system is put into implementation. With more knowledge being acquired in the project, the tool should be improved step by step.

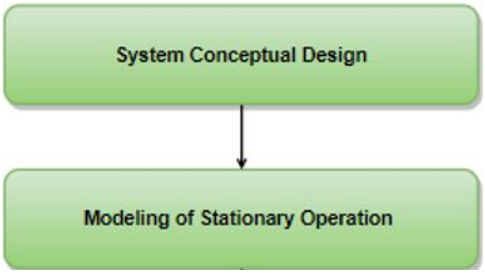
1.3 Study of this master thesis

From the discussion in the previous sections, it can be concluded that the main research question of "Tandem FC in Marine Application" project is: **is the tandem fuel cell system a viable alternative to marine LNG engine power plants?**

To answer this main research question, sub-questions should be answered one by one to pave the way. Since this master thesis is the first study of the whole project, the sub-questions to be answered are:

- Can the efficiency of more than 60% of the tandem fuel cell system as reported in previous research be re-produced?
- Is the transient behavior of the system good enough to be equivalent to or even outperform the marine LNG engine power plants?
- How can the design assistant tool help in the design phase of the system?

To answer the first research question, the steps according to **Figure 1-2** are:



The conceptual design of the system has been proposed in the research assignment (Zhao, 2017), which is shown in **Figure 1-3**.

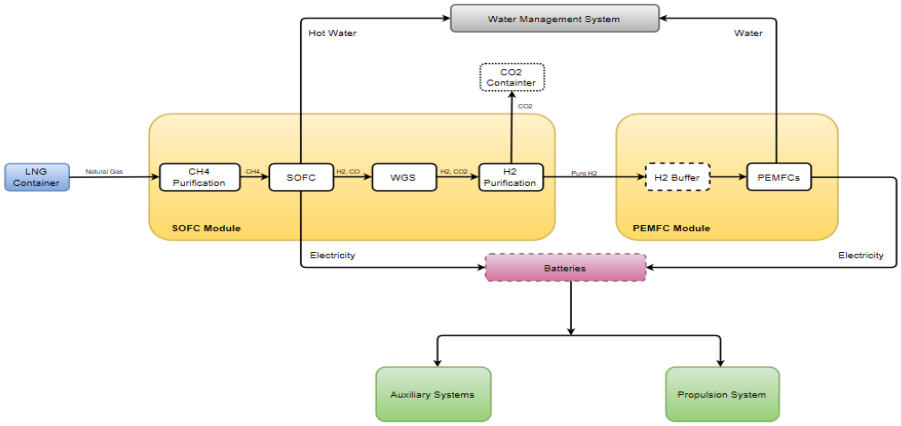


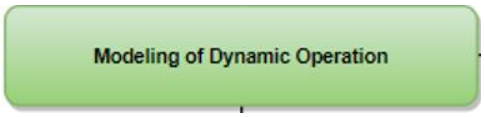
Figure 1-3 Conceptual layout

As can be seen in the system layout, there are two main modules in the system, namely SOFC module and PEMFC module. The SOFC module includes the SOFC system and the gas processing system, and the PEMFC module consists of PEMFC system and a hydrogen buffer, which functions as an energy buffer. At the stage of the research assignment, it was not sure yet whether to hydrogen buffer or batteries as energy buffer. Therefore, both of them were presented in the conceptual design layout with dotted line, which means they both have the possibility to present in the system. The purpose of having an energy buffer is to store enough energy for the system to cope with transient when the power output of the PEMFC is not sufficient. It is a method to enhance the transient behavior of the system. However, to answer the first research question, which is mainly about the performance of the

system under stationary performance, it is unnecessary to include energy buffer in to the stationary model. It will be dealt with in the dynamic modeling section.

The performance of the system under stationary operation (including system efficiency) can be calculated from the stationary model in the step of “Modeling the stationary operation”. Cycle-tempo will be used to build up the stationary model.

To answer the second research question, the step needs to take is:



In this step, a dynamic Matlab/Simulink model is going to be built to analyze the transient behavior of the system.

To answer the third research question, the step needs to take is:

In this step, the dynamic model is going to be further developed into a design assistance tool. The functions of the tool will be added according to the requirement (in this study, the main one is to size the tanks, which will be explained in later chapter).

2. Stationary model

As is stated in Chapter 1, before building the dynamic model, a stationary model is going to be built first. This stationary model is built according to the conceptual design proposed in the research assignment. The purpose of building this stationary model is to have a general overview of the system's performance. For this purpose, directly building an elaborated Matlab/Simulink model is unnecessary since that would consume too much time in the process of modeling before the model can be used for simulation. Besides, building a simplified Matlab/Simulink model for this purpose is also not so appropriate, because to which extent the model of each component should be simplified remains an issue. If it is oversimplified, some important characteristics might be missed; while if it is under-simplified, more time would be consumed. One solution for this dilemma is to find a commercial thermodynamic modeling software program, which has been widely used in both industry and academic field, for the same purpose. Building a stationary model in this type of software program needs less detailed modeling because they normally contain many build-in models for different components. Besides, the credibility of the results can be guaranteed since it has already been widely used. In this way, the process of building the stationary model can reach the balance between effective and efficient. There are many available thermodynamic modeling software programs in the market, and each has it pros and cons. After comparing several options, Cycle-Tempo is selected eventually.

According to the User's Manual (3ME Faculty, TU Delft), Cycle-Tempo is a program for thermodynamic modeling and optimization of systems for the production of electricity, heat and refrigeration. Its UI is relatively straightforward and easy to understand. It contains some built-in thermodynamic apparatuses such as heat exchangers, compressors and pumps. It also contains built-in thermoelectric apparatuses such as fuel cells. All of these are the critical apparatuses required in the stationary model. In order to connect the apparatuses, the user can simply draw pipelines between them, and combine them into a system. The user can also choose which type of pipeline to use according to the substance flowing inside, for example gas or liquid. After connecting all the apparatuses, the user can set parameters for each apparatus and pipeline based on requirements. For example, the user can set the power output for a fuel cell, also the pressure loss in the pipeline. Besides, the conditions of the substance flowing in the pipe (for example temperature, pressure and category) at anywhere can also be assigned. Once the parameters being set and the assigned conditions of the substance flow are sufficient, the software will be able to calculate the conditions of the substance everywhere in the system. In addition, the efficiency, power output and energy loss of each part and the whole system can also be calculated. Should there be any error in user's input or calculation process, the software will give warnings or stop the calculation.

According to the brief introduction above, the advantages of this software can be concluded: first of all, there are many built-in apparatus models that can be directly used. Those built-in models, although simple, are able meet the requirement for stationary modeling; second, the system schemes are simple and straightforward and are convenient to modify and change; finally, the capabilities of calculating the stationary properties (power, efficiency etc.) are sufficient to meet the requirement for the first stage of the study.

Through applying Cycle-Tempo into the stationary modeling, some disadvantages of this software are also observed: first, the software cannot import or export data from external sources. The user has to

deal with these data manually, which can be rather time consuming once the amount of the data is large. Besides, the software is not so stable, which experiences crashes often. Some of those crashes will happen when the user performing some certain operations. However, several of these operations are necessary. Therefore, some relatively tricky ideas have been come up with in order to avoid the operations that will cause crashes. Unfortunately, these ideas always either make the system more complex or add more manual works in data import and export.

In conclusion, although Cycle-tempo has some limitations and shortcomings, it is still appropriate to fulfill the requirement for the first stage of the study due to its convenience and specialization in stationary calculation. The details of the components being used in the model, the subsystems being built and the assumptions being made in the modeling process will be fully described in the upcoming chapters.

2.1 Component details

2.1.1 Fuel cells

One of the main advantages of Cycle-tempo is that it contains a built-in fuel cell model. This model is able to perform stationary calculation for five types of fuel cells. In this study, only SOFC (DIR) as well as PEMFC are going to be used.

2.1.1.1 SOFC (DIR) Model

SOFC (DIR) is short for Solid Oxide Fuel Cell (Direct Internal Reforming), which is the chosen type of SOFC for the tandem fuel cell system. There are two types of internal reforming: Direct Internal Reforming (DIR) and Indirect Internal Reforming (IIR). The reason for selecting DIR is mainly because no other gas processing equipment is required for the first step of gas reforming. Besides, a decent thermal coupling can be achieved at the anode. More details can be referred to in the research assignment report (Zhao, 2017). The basic layout of a SOFC (DIR) is shown **Figure 2-1**. The technical details of the model are to be introduced in detail.

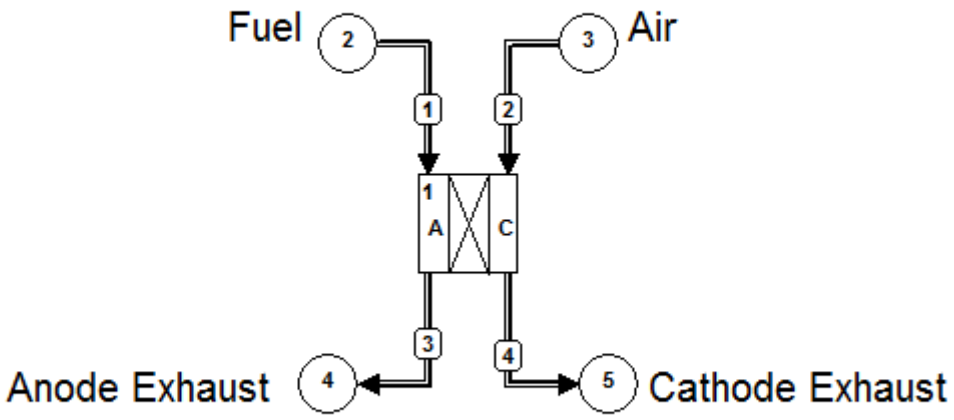


Figure 2-1 SOFC (DIR)

A. As a generator

A.1 Calculating of basic characteristics

The model being used in Cycle-tempo to calculate the characteristics of the SOFC is called the “isothermal model”. (De Groot, 2004) In this model, the main assumption being made is that the concentrations of the gas components are place dependent, while the temperature is fixed. Based on this assumption, this model can not only avoid iterations, but also maintain a relative high accuracy in the calculation. The calculation details and comparison of this model with a detailed model can be found in (De Groot, 2004).

A.2 Input data

For a SOFC model, there are basically two types of inputs: Design condition inputs, and Off-design condition inputs. In design condition, the size of the fuel cell needs to be determined based on the initial requirements (the nominal voltage, current density and power); in off-design condition, the size

of the fuel cell is fixed, and the operational point at which the fuel cell operates can be changed.

For both design condition and off-design condition, the following data always need to be input as an initial condition for the fuel cell:

1) Anode and cathode gas input pressure (PINAN, PINCA);
2) Anode and cathode gas output pressure (POUTAN, POUTCA);
3) Temperature of the fuel cell (TFCELL);
4) Output temperature of the gases (TOUTPS);
5) Fuel utilization factor (UFL).

The input interface is shown in **Figure 2-2**.

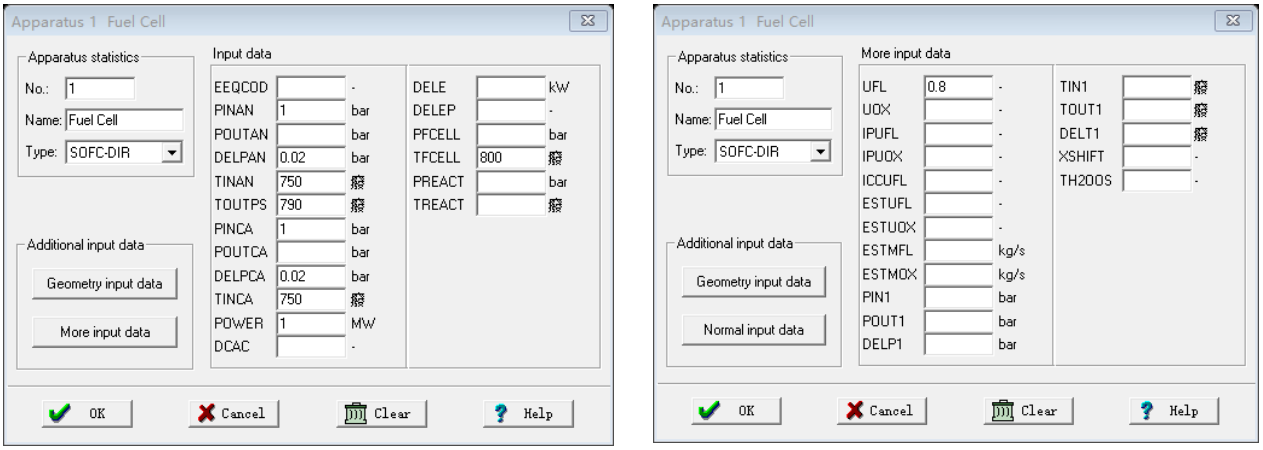


Figure 2-2 Input interface of SOFC (DIR)

Design condition

For design condition, the size of the fuel cell (active cell area A_{FC} (ACELL) and the equivalent cell resistance R_{eq} (RCELL)) needs to be decided based on the requirement. Therefore, in this case, the nominal cell voltage (VCELL) and current density (CDENS) should be specified. The nominal power also needs to be specified in order to calculate the active cell area A_{FC} and the equivalent cell resistance R_{eq}. The input interface of design condition is shown in **Figure 2-3**

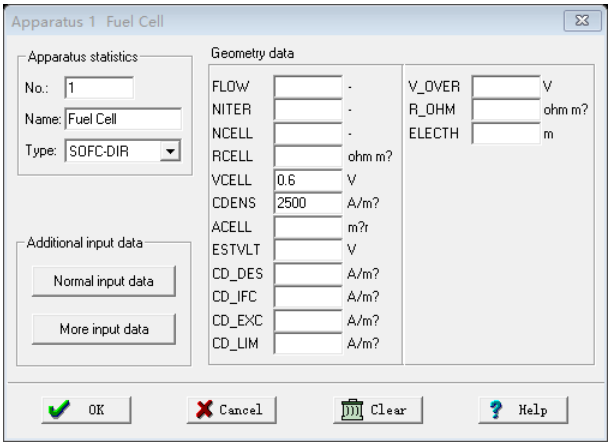


Figure 2-3 Design condition input

Off-design condition

After the size of the fuel cell has been decided, one can change the inputs for the fuel cell in order to simulate its performance under different off-design operational condition. These changeable inputs include power, fuel input, and fuel utilization factor.

B. As direct internal reformer

Apart from generating electric power, another important role that the SOFC plays in the tandem fuel cell system is a reformer, which converts the fuel (Natural Gas) into hydrogen and carbon monoxide. The reaction equation is:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \qquad \text{(reaction 1)}$$

This reaction is known as the reforming reaction, which is taking place simultaneously with the electrochemical reactions in an actual direct internal reforming SOFC. In Cycle-tempo, for the convenience of calculation, the DIR SOFC is modeled in a different manner from the actual process, but the calculated performance is shown to agree quite well. (De Groot, 2004)

In Cycle-tempo, the reforming reaction and the electrochemical reactions are modeled separately, as is shown in **Figure 2-4**. In the first step, the reforming reaction reaches equilibrium. The concentrations of each gas component are calculated based on this equilibrium point. The heat being generated in this step is also calculated. In the second step, the composition of the gas from step one will become the input of the electrochemical reaction. The calculation of the electrochemical reaction is based on the "isothermal model".

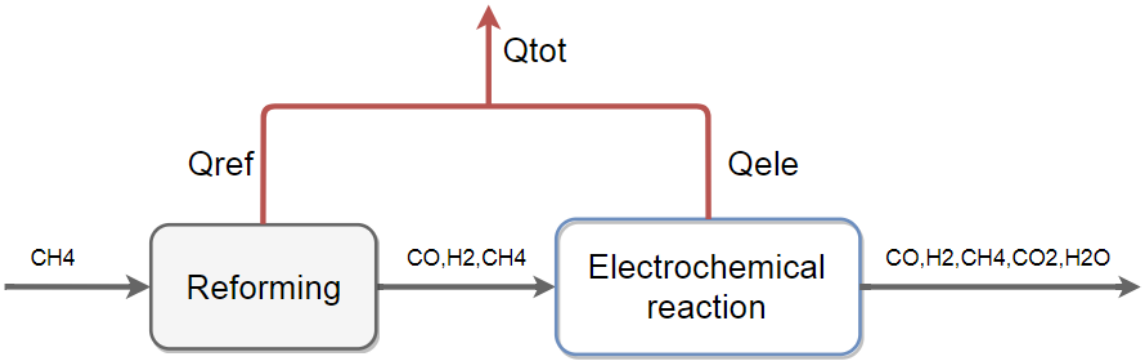


Figure 2-4 SOFC(DIR) working principle in Cycle-Tempo

The composition of the gas flowing out from the chemical reactor is taken as the composition at equilibrium. This is also a reasonable assumption being made in the stationary study stage. Since the fuel cell is going to operate at a constant operational point, it is unnecessary to take kinetics into account. In the case of direct internal reformer, the equilibrium temperature of the chemical reformer is the same as the temperature of the fuel cell. The calculation is performed based on reaction constant, which will be described in **Chapter 2.1.4**.

C. Mass and energy balance

In order to perform calculation, equations that represent the balances of the apparatus need to be used. In the case of an SOFC model, mass balance and energy balance are the equations on which calculations are based.

First, the overall mass balance of this SOFC model is added, which is rather straightforward. It is simply "total-in equals to total-out":

$$\Phi_{m,a,in} + \Phi_{m,c,in} - \Phi_{m,a,out} - \Phi_{m,c,out} = 0 \qquad (2.1)$$

Where $\Phi_{m,a,in}$ and $\Phi_{m,a,out}$ are the input and output the anode, and $\Phi_{m,c,in}$ and $\Phi_{m,c,out}$ are the

input and output of the cathode.

Furthermore, the nature of an operating SOFC is that the oxygen ions goes from the cathode to the anode, therefore, there will be mass exchange between the anode and the cathode, which can be denoted as $\Phi_{m,c\to a}$. This can be expressed as:

$$\Phi_{m,a,out} - \Phi_{m,a,in} = \Phi_{m,c\to a} \quad (2.2)$$

Anode mass flow

The anode mass flow $\Phi_{m,a,in}$ can be specified by users, while in other cases, it is the character to be calculated. In these cases, the electrical power output of the fuel cell should be specified as the initial condition. The $\Phi_{m,a,in}$ will be calculated based on energy balance. That is:

$$\Phi_{m,a,in} \cdot \mu_f \cdot \eta_{DC/AC} \cdot \eta_{SOFC} \cdot LHV_{fuel} = P_{FC} \quad (2.3)$$

Where,

P_{FC} is the power output of the fuel cell (KW);

μ_{fuel} is the fuel utilization factor (-);

$\eta_{DC/AC}$ is the efficiency of DC/AC conversion (-);

η_{SOFC} is the electric efficiency of the SOFC (-);

LHV_{fuel} is the lower heat value of the fuel (KJ/kg)

Cathode mass flow

Similar to anode mass flow, the cathode mass flow also can be either directly specified or calculated from other specifications. In the case of SOFC, this can be realized through specifying the outlet gas temperature of the fuel cell.

In practice, it is more realistic to control the outlet temperature of the fuel cell, because high temperature fuel cells are very sensitive to temperature changes. Too much temperature gradients between the inlet and outlet will lead to damage of the electrode. Therefore, the outlet temperature of the fuel cell should be constantly monitored and controlled. In other words, specifying outlet temperature is more practical than specifying the cathode mass flow. Thus, in the Cycle-tempo model, the outlet temperature is to be specified for the calculation of cathode mass flow.

Once the outlet temperature is specified, the Cycle-tempo model will be able to calculate the cathode input mass flow as well as the oxidant utilization based on energy balance:

$$\Phi_{m,a,in} \times \mathrm{h}_{a,in} + \Phi_{m,c,in} \times \mathrm{h}_{c,in} - \Phi_{m,a,out} \times \mathrm{h}_{a,out} - \Phi_{m,c,out} \times \mathrm{h}_{c,out} = \mathrm{P}_{DC} + Q \quad (2.4)$$

Where

$\mathrm{h}_{a,in}$ is the specific enthalpy of anode gas input (KJ/kgs);

$\mathrm{h}_{c,in}$ is the specific enthalpy of cathode gas input (KJ/kgs);

$\mathrm{h}_{a,out}$ is the specific enthalpy of anode gas output (KJ/kgs);

$\mathrm{h}_{c,out}$ is the specific enthalpy of cathode gas output (KJ/kgs);

P_{DC} is the electric power generated by the SOFC (KW);

Q is the heat generated by the SOFC (KW).

In SOFC, the cathode mas flow is also closely related to cooling issues because air cooling is the mostly used cooling method for SOFCs, which is, therefore, the cooling method to be modeled in the stationary model. Air cooling in SOFC is that the fuel cell will be cooled by the air flow going through

the cathode. Depending on the relationship between the fuel flow and the air flow, the cooling method can be co-flow cooling, counter-flow cooling, and cross-flow cooling. Different flow type will result in different cooling effect. The working principle of the air cooling in SOFC is the same as that of heat exchangers, which will be explained in ***Chapter 2.1.2***.

In practice, both co-flow and counter-flow air cooling can be applied, but they both have their pros and cons: for co-flow, the most outstanding advantage is that the temperature difference between air and fuel along the cell is low. Therefore, it will be less likely to render damage caused by local temperature difference. The local temperature characteristics of both co-flow and counter-flow air cooling are shown in **Figure 2-5**. It can be noticed that the temperature difference between fuel and air in co-flow case is much lower than that in counter-flow case. However, when taking the local voltage character into account, co-flow cooling turns out to be worse counter-flow cooling. See **Figure 2-6**. Counter-flow cooling will result in more steady Nernst potential along the axial, while the Nernst potential of co-flow cooling fuel cells varies a lot. In terms of operating, a steady Nernst potential is certainly more desirable.

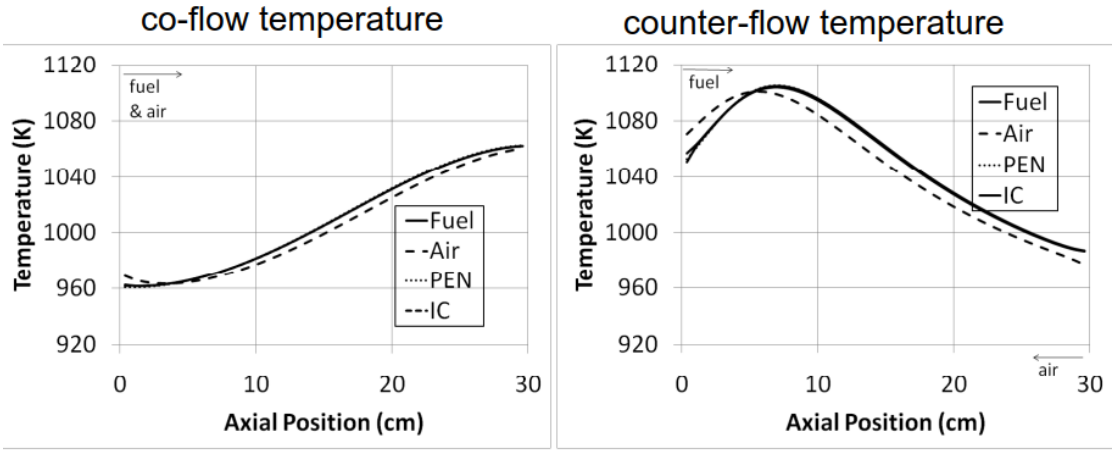


Figure 2-5 Temperature characteristics of co-flow and counter-flow cooling *(J. D. Powers, 2009)*

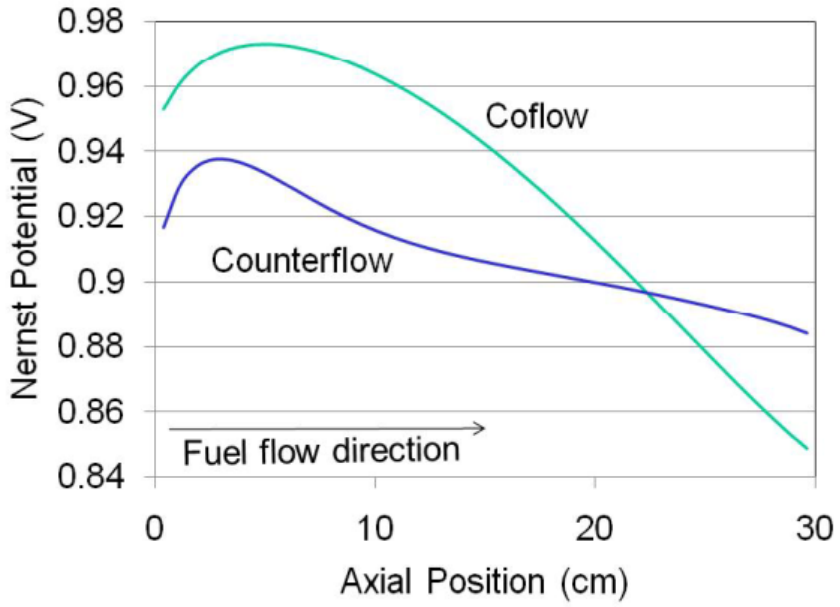


Figure 2-6 Voltage characteristics of co-flow and counter-flow cooling *(J. D. Powers, 2009)*

Above all, it can be concluded that if the local temperature difference between the fuel and air can be limited within a certain range where damage will not occur, then counter-flow will be a better choice than co-flow. According to literatures (P. Pianko-Oprych, 2015) (M. Peksen, 2013), a temperature difference of 100°C will be far lower than causing material damage in SOFCs. In the case of counter-flow cooling, for fuel flow, the highest temperature will occur at the outlet, while for air flow, the lowest temperature is at the inlet, which is, in counter-flow case, the outlet position of the fuel flow. Therefore, if the temperature difference at this position (the outlet of the fuel flow and the inlet of the air flow) can be controlled below 100°C, then damage will not occur. In other words, if low temperature difference at this position is specified to be lower than 100°C, counter-flow air cooling can be selected. In Cycle-tempo, this can be realized by directly specifying the outlet and inlet temperature of the fuel flow and the air flow. Therefore, counter-flow cooling is going to be selected in the Cycle-tempo model. The specification details are listed in **Chapter 2.2.1**.

Gas specific enthalpy

In Cycle-tempo, the specific enthalpy of gas at different temperature can be calculated. For each gas component, the specific enthalpy is calculated by taking into account the standard enthalpy of formation. The reason behind this and how the specific enthalpy is calculated will be described in ***Chapter 3***.

For gas mixtures, apart from temperature, the specific enthalpy will also be influenced by the composition as well as the fraction each component. In Cycle-tempo, all of these factors are taken into consideration by applying Least-Squares Coefficients method (Sanford Gordon, 1994), which is also known as Shomate Equation. The concept of this method and calculation examples will also be given in ***Chapter 3***.

2.1.1.2 PEMFC model

Although The working principle of PEMFC and SOFC differs a lot (for PEMFCs, protons are transferred from the anode to the cathode, while for SOFCs, oxygen ions are transferred from the cathode to the anode), this fact, however, does not result in different the mass balance and energy balance for the two fuel cell types. Therefore, the approach of calculating the basic characteristics (such as current, voltage, power, efficiency, etc.) are the same. And the procedure of sizing in design condition and changing the inputs in off-design condition are also the same. There are only two main differences that worth explaining here.

First of all, unlike SOFC, humidification is a vital consideration for PEMFCs. This is because the membrane in a PEMFC has to be sufficiently moist in order to transport protons properly. Low humidity of the membrane may lead to malfunction or even membrane damage. Therefore, humidification system should be employed prior to the PEMFC to humidify the inlet gas. This might need to be considered when modeling the PEMFC system.

Apart from the need for humidification system, high humidity requirement also makes it impossible for PEMFCs to use air cooling. The physics behind this is that while taking away heat, cooling air flow will also take away a considerable amount of water from the membrane. This may render the humidification system hardly to meet the humidity demand and lead to drought in the membrane. Therefore, in Cycle-tempo, the only available cooling method for PEMFC is water cooling. The system layout of a water cooling PEMFC is shown in **Figure 2-7**.

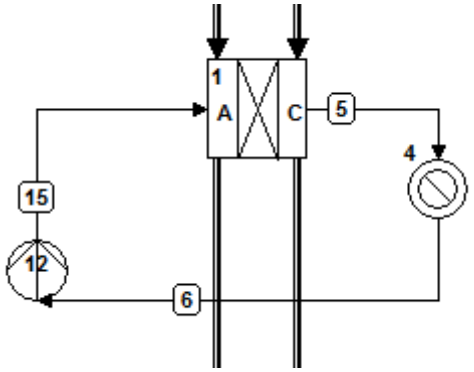


Figure 2-7 PEMFC with water cooling

Although a water cooling system can alleviate the pressure of the humidification system, it adds more complexity to the system. Besides, the relatively low temperature (60-70℃) of the outlet cooling water results in a low thermal quality.

Since air cooling is not selected, Cycle-tempo will not be able to calculate the oxidant utilization (UOX) based on the specified outlet temperature. Therefore, this parameter must be defined by the user. According to literature, a value of around 50% (Eberle Ulrich, 2011) is observed in practice, which will be used in the PEMFC model.

2.1.2 Heat exchangers

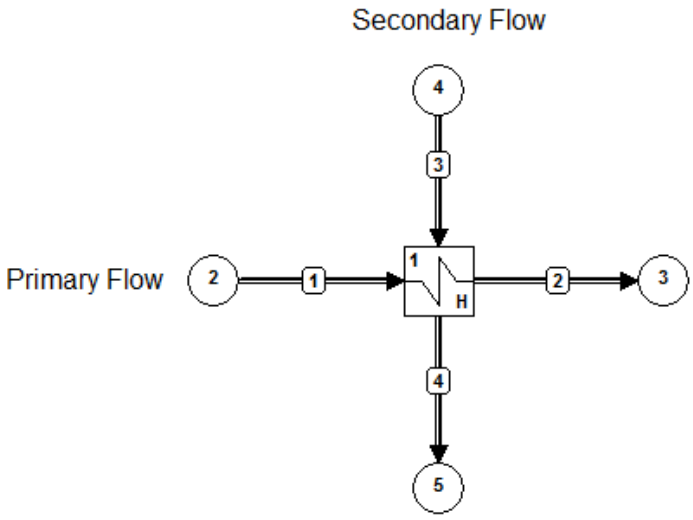


Figure 2-8 Heat exchanger

Heat exchangers are widely used in the tandem fuel cell model, especially in the SOFC subsystem and the Gas Processing subsystem, where considerable amount of waste heat can be recovered. In Cycle-tempo, the built-in heat exchanger model is able to calculate both the temperature of inlets and outlets, and the required mass flow based on the mass balance and the energy balance equations.

The mass balance equations used in the calculation are:

$$\Phi_{p,in} = \Phi_{p,out}$$
$$\Phi_{s,in} = \Phi_{s,out} \quad (2.5)$$

Where

$\Phi_{p,in}$, and $\Phi_{p,out}$ are the inlet and outlet of the primary flow (the flow to be cooled, kg/s);

$\Phi_{s,in}$ and $\Phi_{s,out}$ are the inlet and outlet of the secondary flow (the flow to be heated, kg/s).

The energy balance equation used in the calculation is:

$$\Phi_{p,in} * \mathrm{h}_{p,in} + \Phi_{s,in} * \mathrm{h}_{s,in} = \Phi_{p,out} * \mathrm{h}_{p,out} + \Phi_{s,out} * \mathrm{h}_{s,out} \quad (2.6)$$

Where

$\mathrm{h}_{p,in}$ and $\mathrm{h}_{p,out}$ are the specific enthalpy of the primary inlet and outlet flow (KJ/kgs);

$\mathrm{h}_{s,in}$ and $\mathrm{h}_{s,out}$ are the specific enthalpy of the secondary inlet and outlet flow (KJ/kgs).

Once adding up **equation (2.5)** and **equation (2.6)**, there will be six values left. By knowing any five of them, the one left can be calculated. If the one to be calculated is a mass flow, the EEQCOD should be specified as 1; if the one to be calculated is a temperature, the EEQCOD should be specified as 2.

2.1.3 Compressors and pumps

Figure 2-9 Compressor

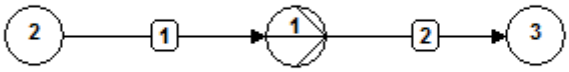


Figure 2-10 Pump

Compressors and pumps are also widely used in the model. They will be employed to drive the gas flows and the liquid flows. Compressors will also be used to pressurize the gas.

Calculations regarding compressors and pumps are based on energy balance:

$$P_{ele} * \eta_{ise} * \eta_{mech} * \eta_{ele} = m * (h_{out} - h_{in}) \quad (2.7)$$

Where,

P_{ele} is the total electric power consumption (KW);

η_{ise} is the isentropic efficiency (-);

η_{mech} is the mechanical efficiency (-);

η_{ele} is the electrical efficiency (-);

m is the mass flow (kg/s);

h_{out} is the specific enthalpy of the outlet flow (KJ/kgs);

h_{in} is the specific enthalpy of inlet flow (KJ/kgs).

In this study, for both compressors and pumps, η_{ise} is set to be 0.8. (Stephen, 2012) , which is in the middle of the efficiency range of a well-designed compressor or pump (0.75-0.85). As to the electrical efficiency and the mechanical efficiency, if not specified by the user, their value will be taken from a regression curve based on empirical data. The curve is shown in **Figure 2-11**.

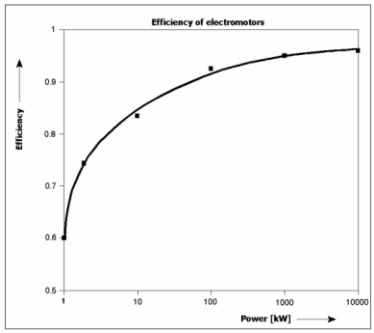


Figure 2-11 Mechanical efficiency and electrical efficiency of compressors and pumps as a function of power *(3ME Faculty, TU Delft)*

The efficiency on the vertical axis is the production of mechanical efficiency and electrical efficiency, and the power on the horizontal axis is the nominal power of the compressor or pump. Since the data for making the curve are from real motors, and for the simplicity of the modeling process as well, the value of mechanical efficiency and electrical efficiency will be ones from interpolation of **Figure 2-11**.

2.1.4 Chemical reactors

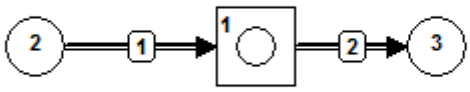


Figure 2-12 Chemical reactor

Chemical reactors will be used in the two-step water gas shift in the Gas Processing subsystem. Water gas shift reaction is one of the two built-in reactions that Cycle-tempo can directly perform calculation with. The reaction equation is given by:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \text{(reaction 2)}$$

The calculations are performed under equilibrium state (the reason for this assumption is the same as the one described in the SOFC(DIR) model), and the equilibria is calculated by means of equilibrium constant, which is a function of temperature.

$$K_{reaction} = f(T_{reaction}) \qquad (2.8)$$

Where,

$K_{reaction}$ is the equilibrium constant of the reaction (-);

$T_{reaction}$ is the temperature at which the equilibrium is calculated (K).

The temperature at which the reaction takes place can be specified by the user. The calculation of the partial pressure (mole fraction) of each gas component under equilibrium is done based on **equation (2.17)**:

$$\frac{(\partial P_{CO_2} + x)(\partial P_{H_2} + x)}{(\partial P_{CO} - x)(\partial P_{H_2O} - x)} = K_{reaction} \qquad (2.9)$$

Where,

∂P is the partial pressure of the component (bar);

x is the reaction coordinate of the reaction.

Given the partial pressure of each gas component (CO_2, H_2, CO, H_2O) of the inlet gas, and the temperature at which the reaction takes place, Cycle-tempo can calculate the value of x (it is able to automatically filter out the inappropriate root, that is the negative root). By adding the value of x to the partial pressure of each component, the new gas composition can be acquired.

2.1.5 Separators

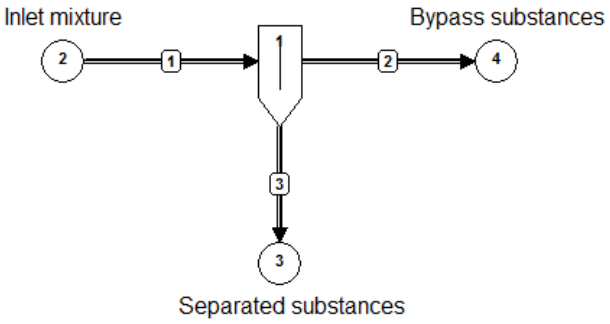


Figure 2-13 Separator

Separators are employed in the gas processing system for the purpose of separating ceratin gas components from the gas mixture after the two-stage water gas shift reactions. The working principle of this apparatus is rather simple: the separated substances stay, while the bypass substances pass through. In Cycle-tempo, not only the type of the separated substances and the bypass substances can be specified, but also the effectiveness of the separator can be adjusted by the user. The effectiveness of the separator is given by the mass flow of the separated substance divided by the total mass flow of the substance to be separated in the gas mixture. For instance, consider this case: the inlet gas mixture is composed by 90% N2 and 10% CO, the mas flow is $1kg/s$, the effectiveness of the separator is 90%, and CO is to be separated. Then the mass flow of the separated substance will be:

$$1\,kg/s * 10\% * 90\% = 0.09\,kg/s$$

The settings of the separated substances and the effectiveness will be described in the next chapter when separators are used in the gas processing subsystem.

2.2 Subsystems

2.2.1 SOFC system

As is mentioned in the previous chapter, the SOFC operates both as a generator and a natural gas reformer. As can be seen in **Figure 2-14**, natural gas and air are fed in to the system, while cathode exhaust and syngas come out from the system. Meanwhile, electricity is generated by the SOFC. The syngas contains CO and H_2O, which will become the reactants of water gas shift (WGS) reactions taking place in the next subsystem (gas processing system).

The SOFC operates at high temperature, which means fuel gas and air should also be fed at high temperature. Otherwise, damage may occur at the inlets because of huge temperature difference. Therefore, preheating of the gases is required. Fortunately, when operating, the SOFC will generate a considerable amount of heat, which, in the case of SOFC, will be taken away by cooling air flow. (As is mentioned before, air-cooling of the SOFC is realized by feeding excessive air at the cathode.) Since the temperature of the outlet cooling air flow also needs to be maintained high in order to avoid large temperature gradients, high thermal quality can be expected from cathode exhaust gas flow. Therefore, the idea of using cathode exhaust gas as a heating source for the inlet gases came into being. Apart from cathode exhaust gas, the syngas going out from the anode also contains a high thermal quality, and can also be used as a heating source. However, since the syngas is the reactant for the high temperature water gas shift (WGS) reaction, whose temperature requirement is 350°C, in the gas processing system after the SOFC system, the heat that can be taken advantage of from the syngas is limited. Compressors are needed to drive the gas. The system sketch of this system is shown in **Figure 2-14**.

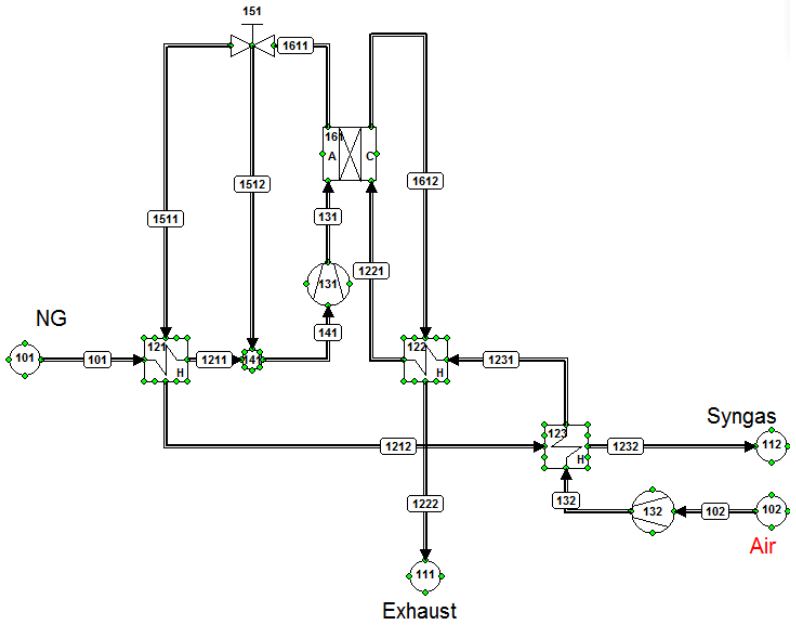


Figure 2-14 SOFC System

As can be noticed that at the anode part, there is a special design for anode gas recirculation. This is for the purpose of enhancing the overall system efficiency. By recirculating part of the anode exhaust gas, the heat can be recovered (Biert, Godjevac, Visser, & Aravind, 2016). Also, the steam in the anode exhaust gas can be reused as reactant for the internal reforming reaction. In this way, no extra

steam source is required. According to (D. Saebea, 2015), when the recirculation percentage is selected as 40%, the SOFC can achieve the highest electrical efficiency.

The basic parameters of each apparatus are shown in the **Table 2-1**. Since for the current study scope, the interaction between the system and the surroundings is not considered, it is assumed that there is no heat exchange between the system and the environment. Also, losses in the pipes are assumed to be zero. These assumptions are also applied to the parameter settings of the GPS subsystem and the PEMFC subsystem.

Sources				
Gas	**Composition (mole fraction)**		**POUT (bar)**	**TOUT (°C)**
NG (101)	CH4 81.29%, N2 14.32%, C2H6 2.87%, Others 1.52%		1.01325	15
Air (102)	N2 77.29%, O2 20.75%, H2O 1.01%, Ar 0.92%, CO2 0.03%		1.01325	15
Heat exchangers				
Number	**EEQCOD**	**DELP1 (bar)**	**DELP2 (bar)**	**TOUT (°C)**
121	2	0.02	0.02	-
122	2	0.02	0.02	-
123	2	0.02	0.02	350
Compressors				
Number		**ETHAI**		
132		0.8		
133		0.8		
Valve				
Number	**Pipe to specify flow for**		**Flow**	**Flow relative to pipe**
151	1512		0.4	1611
Fuel cell				
Number	**EEQCOD**	**DELTP (bar)**	**TIN (°C)**	**DC/AC**
161	1	0.02	750	0.96
TOUT (°C)	**TCELL (°C)**	**PCELL (bar)**	**IPUFL**	**PINAN, PINCA (bar)**
800	800	1	1211	1.15

Table 2-1 SOFC system settings

2.2.2 Gas Processing system

Although the direct internal reforming SOFC can convert CH_4 into H_2, CO will also be generated as a byproduct (see **reaction 1**). Since the PEMFC can only use H_2 as fuel and CO is toxic for its membrane, the CO component in the syngas coming out from the SOFC system has to be removed. And that is why the Gas Processing System is employed.

The Gas Processing System contains two sections: the water gas shift (WGS) section and the pressure swing adsorption (PSA) section. In the WGS section, water gas shift reactions take place, and thanks to them, the CO in the syngas coming out from the SOFC system can not only be removed, but also converted into H_2, which significantly increases the overall H_2 production. The reaction equation of WGS is given in **reaction 2**.

The WGS reaction is moderately exothermal, and the heat generated can be recovered. In this case, the heat is used to evaporate water and produce steam.

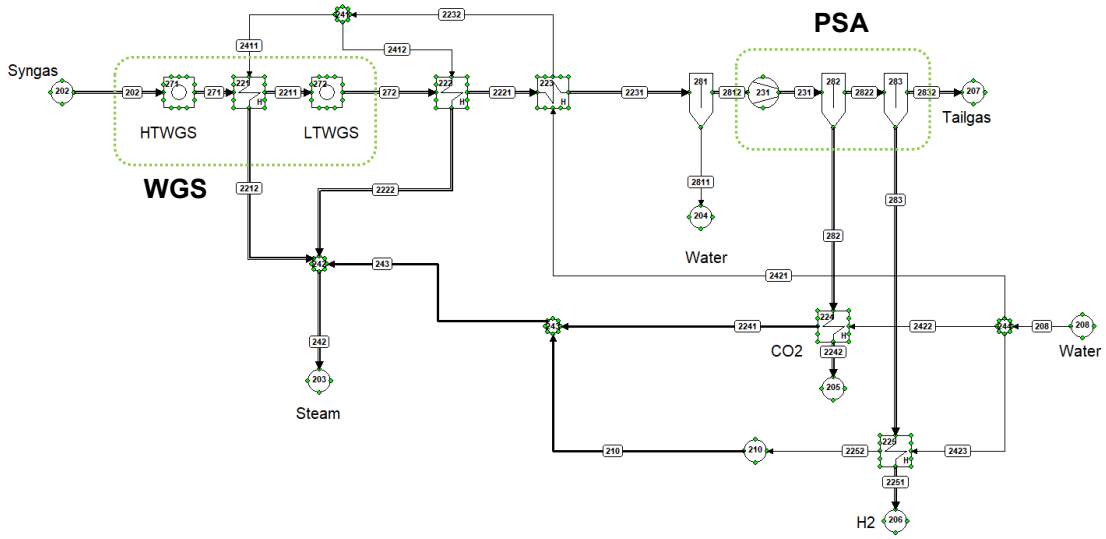


Figure 2-15 Gas processing system

As can be noticed in **Figure 2-15**, there are two WGS reactors in the WGS section. The first one operates at 350°C, while the second operates at 200°C This is actually an approach to recover more H_2. The theory behind is: first, since **reaction 2** is an exothermal reaction, when the temperature is higher, there will be less H_2 being produced, because the equilibrium of an exothermal reaction will move to the left when temperature increases. However, low temperature will limit the reaction rate, which means although a low temperature reactor can convert more CO into H_2, the converting rate will be so slow that may not meet the requirement of H_2 production. Having these two considerations in mind, the necessity of applying two stage WGS can be seen: first, the high temperature WGS reactor converts the syngas which contains a large amount of CO at a high rate. However, because of the limitation of equilibrium, a small amount of CO will still come out from the high temperature WGS reactor. The low temperature WGS reactor will then start to play the role of further converting the remaining CO. Since the amount of CO in the syngas coming out from the high temperature WGS reactor is not as large as that from the SOFC system, the requirement for reaction rate is not an issue for the low temperature WGS reactor anymore. In this way, the requirement for both high converting speed and high conversion rate can be fulfilled.

As is shown in **reaction 2**, although CO can be removed in WGS reactions, unwanted CO_2 is produced. Besides, because of the reversibility of the reaction, tiny amount of CO will still present in the gas coming out from the low temperature WGS reactor, which can still be toxic for the PEMFC. All of these factors contribute to the employment of the PSA system.

Different from WGS, PSA is completely a physical process. It takes advantage of the fact that different gases behave differently under pressure changes. By sharply changing the pressure of the gas mixture, different components can be separated. The detailed working principle can be referred to in **(http://www.oxymat.com/pressure-swing-adsorption-psa-technology/)**. After the PSA section, the purity of the acquired hydrogen can reach as high as 96% (Ole Marius Moen, 2014), which is high enough for meeting the requirement of PEMFCs.

Since there is no built-in model in Cycle-tempo for PSA, it has to be modeled with other built-in models. As is mentioned above, the PSA is essentially a physical separator which separates gases by means of changing pressure. Therefore, as is shown in **Figure 2-15**, it is reasonable to be modeled as a compressor and several physical separators.

The basic parameters of each apparatus are shown in the **Table 2-2**.

Source					
Type		**POUT (bar)**		**TOUT (°C)**	
Water (201)		1.01325		15	
Reactor					
Number		**TWGS (°C)**		**DELP (bar)**	
271		350		0.02	
272		200		0.02	
Heat exchangers					
Number	**EEQCOD**	**DELP1 (bar)**	**DELP2 (bar)**	**TOUT1 (°C)**	**TOUT2 (°C)**
221	1	0.02	0.02	200	110
222	1	0.02	0.02	100	110
223	2	0.02	0.02	30	-
224	1	0.02	0.02	20	110
225	1	0.02	0.02	20	110
Compressors and pumps					
Number			**ETHAI**	**POUT (bar)**	
231			0.8	21	
Separators					
Number			**Separated components**		
281			H2O		
282			CO2		
283			H2		

Table 2-2 Gas processing system settings

2.2.3 PEMFC system

Apart from the SOFC, the PEMFC is the other power generator. However, as is introduced in **Chapter 1**, what is expected from one of them is much different from the other. For the PEMFC, its main task in the tandem fuel cell system is to deal with the transient. Since Cycle-tempo is only capable of dealing with stationary modelling, the dynamic characteristics of the PEMFC cannot be studied by using this software. Therefore, only the performance of the PEMFC under stationary operation will be studied in the Cycle-tempo model.

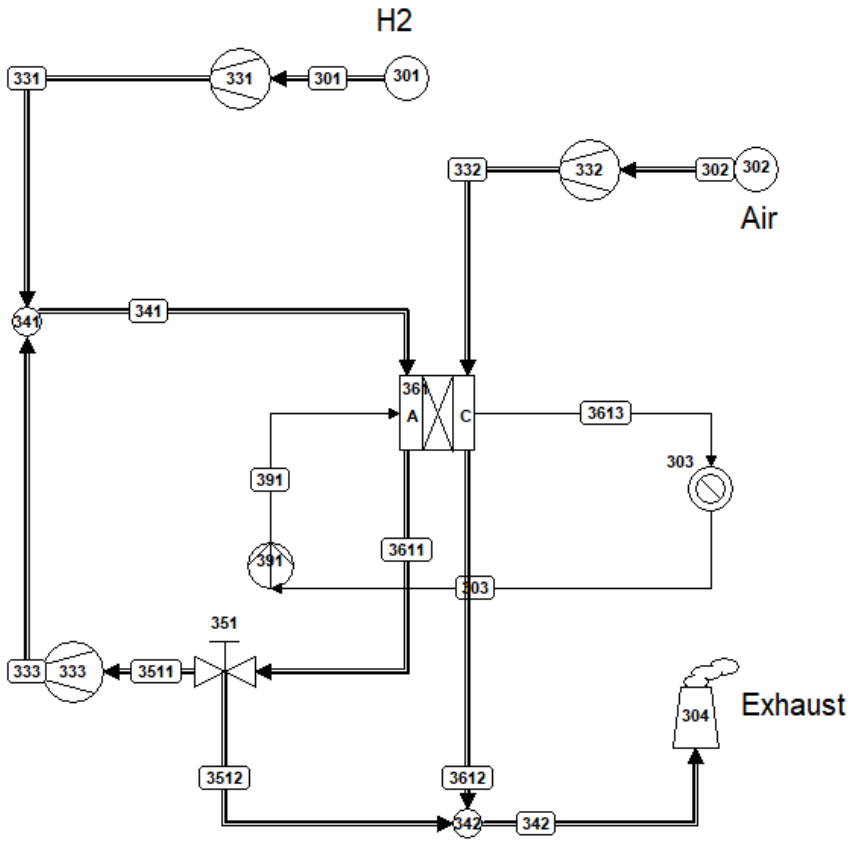


Figure 2-16 PEMFC system

The system sketch is shown in **Figure 2-16**. There are two explanations need to be made here:

(1) As is shown in the system sketch, anode exhaust gas is also recirculated in the PEMFC system. This is also for the purpose of increasing the overall system efficiency by recovering heat from the exhaust gas.

(2) It has been explained in previous chapter that humidification of the PEMFC is of great importance in real operation. However, when considering about the purpose of the Cycle-tempo model, which is only meant for stationary performance study, the humidification system can be discarded. The reasons are: first, the humidification system will not greatly influence the stationary behavior of the system ─ little energy is consumed, and no significant influence on the composition of the gas mixtures except increasing their humidity. Besides, in Cycle-tempo, if the humidity requirement of the PEMFC is not fulfilled, the software will only give warnings in the message window, while the calculation can proceed and the result will be the same as that for sufficient humidity case. Therefore, discarding the humidification system is a reasonable simplification in the Cycle-tempo

model.

The basic parameters of each apparatus are shown in the **Table 2-3**. I

Source			
Type	**POUT (bar)**	**TOUT ($°C$)**	**DELM (kg/s)**
H2 (301)	**1.01325**	**20**	**According to previous stage**
Air (302)	**1.01325**	**15**	**-**
Water (303)	**1.01325**	**15**	**-**

Compressors and pumps:	
Number	**ETHAI**
331	**0.8**
332	**0.8**
333	**0.8**
391	**0.8**

Valve			
Number	**Pipe to specify flow for**	**Flow**	**Flow relative to pipe**
351	**3512**	**0.9**	**3611**

Fuel cell						
Number	**EEQCOD**	**PIN (bar)**	**TOUT ($°C$)**	**PCELL (bar)**	**DELP (bar)**	**TIN ($°C$)**
361	**1**	**1.5**	**70**	**1**	**0.05**	**70**
TCELL ($°C$)	**UFL**	**UOX**	**TOUT1 ($°C$)**	**DELP1 (bar)**	**DC/AC**	
70	**0.95**	**0.5**	**65**	**0.01**	**0.96**	

Table 2-3 PEMFC system setting

3. Stationary model verification

3.1 Background

The verification of the model has been done by means of enthalpy balance, which essentially is energy balance (first law). Because of the presence of chemical reactions in all the three subsystems, the enthalpy of formation of each component of all the gas flows has to be taken into account. Due to the fact that the calculation conventions of enthalpy for chemical engineering and for mechanical engineering are different (especially in terms of signs), the "model verification" section has caused a slight confusion and a short discussion in the midterm meeting. Although finally, a common agreement has been achieved, a more explicit explanation of the enthalpy balance calculation is required in this final report.

3.2 Standard enthalpy of formation

The definition of standard enthalpy of formation of a compound is "the change of enthalpy during the formation of 1 mole of the compound from its constituent element, with all substances in their standard states, and at a pressure of 1 bar and a temperature of 25 $°C$".

When there are chemical reactions taking place in the system, it is a common practice to take into account the enthalpy of formation in the enthalpy balance calculation. In this manner, the heat input and output of the system due to the exothermal and endothermal reactions does not require extra consideration. This is also the way in which energy balance in Cycle-tempo is calculated.

The way how standard enthalpy of formation is taken into account can be described by **equation (3.1)**. The specific enthalpy of a certain gas at temperature T is given by:

$$h_T = [h_f + \int C_P(T)\, d(T - 25°C)] \tag{3.1}$$

In which,

h_T is the specific enthalpy of the gas at temperature T;

h_f is the standard enthalpy of formation of the gas;

C_P is the specific heat of the gas at temperature T;

The values of standard enthalpy of formation h_T for each gas that will exist in the system can be found in **Table 3-1**.

Gas	Enthalpy of Formation (KJ/mol)	Gas	Enthalpy of Formation(KJ/mol)
N2	0	C2H6 (Ethane)	-1560.70
O2	0	C3H8 (Propane)	-2219.22
CO2	-393.52	C4H10 (Butane)	-2877.50
CH4	-74.87	C5H12 (Pentane)	-40.45
H2	0	C6H14 (Hexane)	-53.89
H2O	-285.83	Ar	0
CO	-110.53		

Table 3-1 Standard enthalpy of formation (NIST Chemistry WebBook)

3.3 Calculation of gas specific enthalpy

As can be seen in **equation 3.1**, the specific heat of the gas (C_P) is also influencing the specific enthalpy. C_P varies with temperature, so the relationship between the temperature and C_P has to be known. As is mentioned in **Chapter 2.1.1.1**, in Cycle-tempo, Least-Squares Coefficients method is applied to take in into consideration the influence of temperature to C_P when calculating C_P of the gases. The relationship between the two is given in a polynomial relation in this method. **(NIST Chemistry WebBook)**,

$$C_P(T) = A + B * t + C * t^2 + D * t^3 + E/t^2 \tag{3.5}$$

Where,

T is the temperature of the gas;

$t = T/1000$;

$A - E$ are polynomial coefficients that varies with gas type, which can be found in NIST WEBBOOK.

The specific enthalpy of the gas by definition is the integration of C_P in terms of temperature. Therefore,

$$h = \int C_P(T)\, dT \tag{3.6}$$

Where,

h is the specific enthalpy of the gas.

When expressed in a polynomial form, it becomes:

$$h = A * t + B * t^2/2 + C * t^3/3 + D * t^4/4 - E/t + F \tag{3.7}$$

The integration constant F can also be found in NIST WEBBOOK.

Here is a calculation example:

Calculate the specific enthalpy of hydrogen at 500K.

It can be found in NIST WEBBOOK that when temperature is within the range of 289K-1000K, the polynomial coefficients are:

A	B	C	D	E	F
33.066	-11.363	11.432	-2.773	-0.159	-9.981

Substitute the coefficient into **equation (3.7)**:

$$h_{500} = 33.066 * 0.5 - 11.363 * 0.5^2/2 + 11.432 * 0.5^3/3 - 2.773 * 0.5^4/4 + 0.159/0.5 - 9.981$$

$$h_{500} = 5.883\ kJ/mol$$

Therefore, the specific enthalpy of hydrogen at 500K is $5.883\ kJ/mol$.

3.4 Specific enthalpy of gas mixture

For gas mixtures, the specific enthalpy is given by:

$$h_{mix} = \sum h_i * y_i \tag{3.8}$$

Where,

h_{mix} is the specific enthalpy of the gas mixture;

h_i is the specific enthalpy of one gas component;

y_i is the mole fraction of that component.

3.5 Verification process

First, a stationary operational point of the system has to be found in order to perform the verification. This point can be randomly chosen. In this case, it is chosen as:

$$\Phi_{NG} = 0.1\ kg/s\,;\ UFL_{SOFC} = 0.8$$

3.5.1 SOFC system

The energy balance conceptual figure of the SOFC system is shown in **Figure 3-1.**

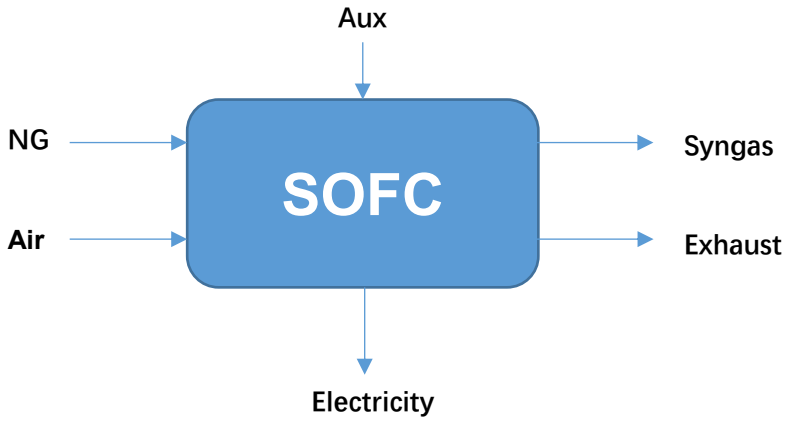


Figure 3-1 Energy balance of SOFC system

As can be seen from **Figure 3-1**, The gas flows going into the system are NG and air, and the ones going out of the system are syngas and Cathode exhaust.

The composition and the temperature of each gas flow are shown **Table 3-2**.

Gas	**Composition (mole fraction)**	**Temperature ($°C$)**
NG	CH4 81.29%, N2 14.32%, C2H6 2.87%, Others 1.52%	15
Air	N2 77.29%, O2 20.75%, H2O 1.01%, Ar 0.92%, CO2 0.03%	15
Syngas	N2 5.14%, H2O 40.96%, CO2 21.84%, CO 10.53%, H2 21.52%	350
Exhaust	N2 78.83%, O2 19.17%, H2O 1.03%, Ar 0.94% CO2 0.03%	82.29

Table 3-2 SOFC system gas composition and temperature

The calculation result is shown in **Table 3-3**:

	Gas	h (KJ/kg)	Mass flow (kg/s)	H (KJ/s)
Input	NG	-3633.23224	0.1	-363.32
	Air	-98.9725471	10.433	-1032.58
	Aux			199.90
			Total	-1196.00
Output	Syngas	-8496.02631	0.326	-2769.70
	Exhaust	-32.6748387	10.207	-333.51
	Fuel cell			1908.29
			Total	-1194.93
			error	1.08

Table 3-3 SOFC system energy balance calculation

As is shown in **Table 3-3**, the error between the input and the output is 1.08 (0.09%), which means the energy balance of the SOFC system model has been verified.

3.5.2 Gas processing system

The energy balance conceptual figure of the gas processing system is shown in **Figure 3-2.**

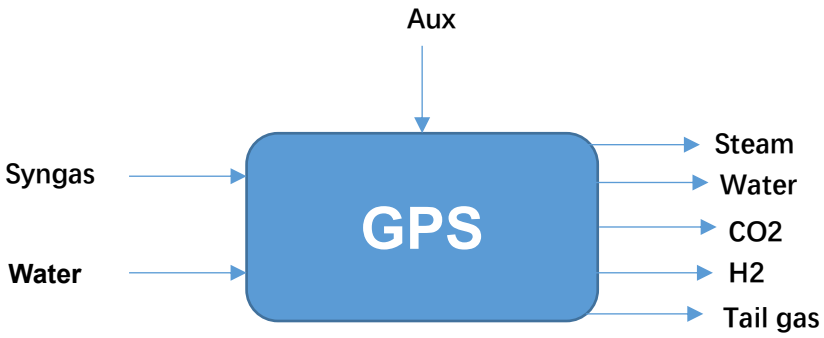


Figure 3-2 Energy balance of gas processing system

What enter the subsystem are the syngas from the SOFC system and liquid water. Steam, liquid water, carbon dioxide, hydrogen as well as tail gas will exit.

The composition and the temperature of each flow are shown **Table 3-4**.

Flow	Composition (mole fraction)	Temperature ($°C$)
Syngas	N2 5.14%, CO2 21.84%, H2O 40.96%, CO 10.53%, H2 21.52%	350
Water (in)	100%	15
Steam	100%	108.19
Water (out)	100%	30
CO2	100%	20
H2	100%	20
Tail gas	CO 2.81%, N2 97.19%	420.25

Table 3-4 Gas processing system gas composition and temperature

The calculation result is shown in **Table 3-5**:

	Gas	h (KJ/kg)	Mass flow (kg/s)	H (KJ/s)
Input	Syngas	-8496.026306	0.326	-2769.70
	water in	-15921.94151	0.132	-2101.70
	Aux			146.59
			Total	-4724.81
Output	Steam	-13278.73665	0.132	-1752.79
	Water out	-15859.08773	0.082	-1300.45
	CO2	-8948.088765	0.212	-1896.99
	H2	-73.50384092	0.01	-0.74
	Tailgas	308.0619464	0.022	6.78
	condense water			222.05
			Total	-4722.14
			error	2.67

Table 3-5 Gas processing system energy balance calculation

As is shown in **Table 3-5**, the error between the input and the output is 2.67 (0.06%), which means the energy balance of the gas processing system model has been verified.

3.5.3 PEMFC system

The energy balance conceptual figure of the PEMFC system is shown in **Figure 3-3.**

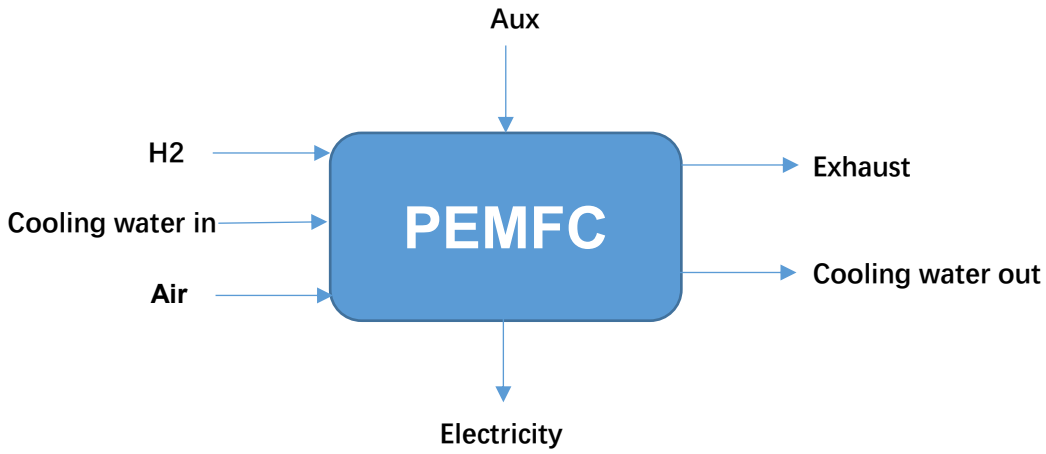


Figure 3-3 Energy balance of PEMFC system

Hydrogen, cooling water and air are entering the PEMFC system, while the exhaust and the cooled cooling water are leaving.

The composition and the temperature of each flow are shown **Table 3-6**.

Flow	**Composition (mole fraction)**	**Temperature ($°C$)**
H2	100%	20
Cooling water (in)	100%	15
Air	N2 77.29%, O2 20.75%, H2O 1.01%, Ar 0.92%, CO2 0.03%	15
Exhaust	H2 0.1%, N2 69.96%, O2 9.39%, H2O 19.7%, Ar 0.83%, CO2 0.03%	70
Cooling water (out)	100%	65

Table 3-6 PEMFC system gas composition and temperature

The calculation result is shown in **Table 3-7**:

	Gas	h (KJ/kg)	Mass flow (kg/s)	H (KJ/s)
Input	H2	-73.50384092	0.01	-0.74
	water in	-15921.94151	2.386	-37989.75
	Air	-98.97254706	0.659	-65.22
	Aux			33.41
			Total	-38022.30
Output	Exhaust	-1751.434696	0.669	-1171.71
	Water out	-15712.67727	2.386	-37490.45
	Fuel cell			640.59
			Total	-38021.57
			error	0.73

Table 3-7 PEMFC system energy balance calculation

As is shown in **Table 3-7**, the error between the input and the output is 0.73 (0.002%), which means the energy balance of the PEMFC system model has been verified.

4. Stationary model simulation

After the model is built and verified, the stationary model is then able to be used for simulation. Two simulations are going to be run with the stationary model. The first one is to examine how the change in the fuel utilization factor (UFL) of the SOFC will influence the overall performance of the whole system. The reason why the UFL of SOFC is chosen to be the variable in the simulation is due to the working principle of the tandem fuel cell system. When the UFL of SOFC is higher, the SOFC can operate at higher power output, since more fuel is converted into electric power. However, this will result in decrease in the amount of hydrogen being generated, which means the power output of the PEMFC will be lower. In contrast, if the UFL of the SOFC is lower, the power output of the SOFC will be lower, although that of the PEMFC will be higher since more hydrogen is available. This dilemma may result in difference in the overall efficiency of the system. In previous researches, the results show that a low UFL of the SOFC can result in high overall efficiency of the whole system. This study will run simulations under different ULF of SOFC to see whether those results can be reproduced. The second simulation is designed to test the system's performance under different power distribution between the SOFC and the PEMFC. The purpose of this simulation is to pave the way for the dynamic study, in which power distribution is a crucial consideration. This will be elaborately explained in **Chapter 4.2**.

4.1 Simulation 1

This simulation is meant to study how the UFL change of the SOFC will influence the overall performance of the tandem fuel cell system, while providing a general overview of the system's performance. The results from this simulation can be compared with those from (Fernandes, Woudstra, Wijk, Verhoef, & L. Aravind, 2016) to see if similar results can be reproduced.

4.1.1 Design condition

Before testing different inputs and running simulations, several main characteristics of the fuel cells have to be determined based on the assumptions in design condition. For the SOFC, is assumed that it constantly works at 1MW power output condition. The reason for choosing 1MW is only for the convenience of calculation. When it is working at this working point, the cell voltage is 0.7V, and current density is 2500A/m^2. The overall fuel utilization factor is 0.95, which results in a fuel utilization per pass of 0.81. (Fernandes, Woudstra, Wijk, Verhoef, & L. Aravind, 2016)

By inputting these values, Cycle-tempo can calculate the cell active area and equivalent cell resistance, which are 595.24m^2 and $9.45 * 10^{-5}\Omega m^2$. These will be used as inputs in the off-design simulations.

For the PEMFC, it is assumed that the requirement for voltage and current density are 0.7V and 2500A/m^2. (Fernandes, Woudstra, Wijk, Verhoef, & L. Aravind, 2016) It is also assumed that in all the off-design simulations, the PEMFC is with the capacity that just consumes the instantly produced hydrogen from the previous two subsystems. That is, in every off-design case, the PEMFC is sized according to the hydrogen production. Therefore, there is no need to specify the power output of the PEMFC.

4.1.2 Simulation and result

Six groups of simulation have been run in order to study how the fuel utilization factor (UFL) of the SOFC will affect the overall performance of the whole system. The UFL in each group is shown in **Table 4-1.**

Group	S1	S2	S3	S4	S5	S6
Overall UFL	0.8	0.83	0.86	0.89	0.92	0.95
UFL per pass	0.6389	0.6726	0.7071	0.7427	0.7793	0.8170

Table 4-1 Simulation groups

To study the overall performance of the system, the following factors are going to be considered:

(1) Hydrogen production
(2) Carbon dioxide production
(3) Power output of the SOFC and the PEMFC
(4) Auxiliary consumption
(5) Overall power output of the system
(6) Overall efficiency of the system

4.1.2.1 Hydrogen production

The result of hydrogen production of each group is shown in **Table 4-2**, where the mass percentage is equal to $(H_2\ mass\ flow/NG\ mass\ flow)$, and mole percentage is equal to $(H_2\ mole\ flow/NG\ mole\ flow)$

Group	H2 Production (kg/s)	Mass Percentage	Mole Percentage
S1	0.00442	9.61%	89.55%
S2	0.00396	8.61%	80.23%
S3	0.00349	7.59%	70.71%
S4	0.00301	6.54%	60.99%
S5	0.00254	5.52%	51.46%
S6	0.00207	4.50%	41.94%

Table 4-2 Hydrogen production

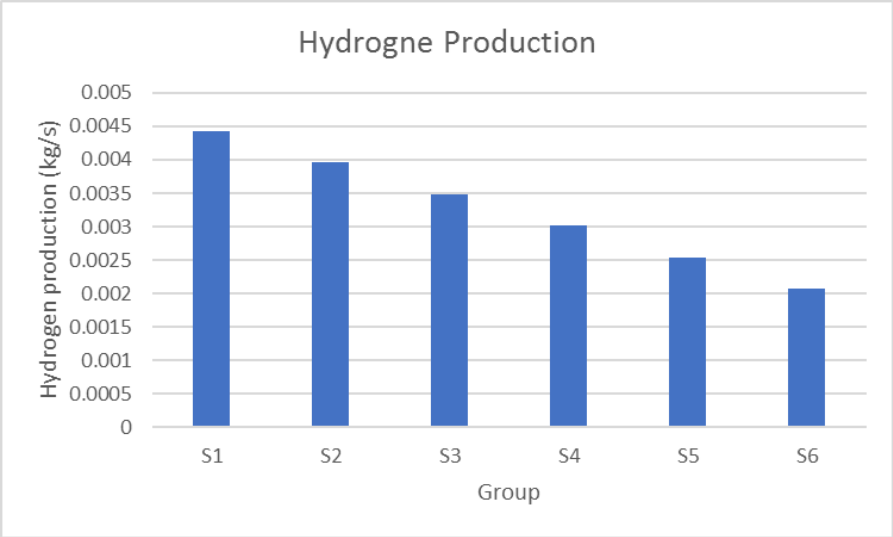


Figure 4-1 Hydrogen production

It can be seen from the table that hydrogen production reduces when UFL is getting higher. This is

also the case for both mass percentage and mole percentage. The reason why mole percentage also increases when reducing UFL is that not all the produced is from the internal reforming of the SOFC. The water gas shift reactions also contribute a lot. With the lower UFL, more CO will be produced from the SOFC. This amount of CO will then become the reactant for water gas shift reaction, which results in higher hydrogen production.

4.1.2.2 Carbon dioxide production

The result of hydrogen production of each group is shown in **Table 4-3**, where the mass percentage is equal to $(CO_2\ mass\ flow/NG\ mass\ flow)$, and mole percentage is equal to $(CO_2\ mole\ flow/NG\ mole\ flow)$

Group	CO2 Production (kg/s)	Mass Percentage	Mole Percentage
S1	0.09751	211.98%	89.80%
S2	0.09773	212.46%	90.00%
S3	0.09794	212.91%	90.20%
S4	0.09770	212.39%	89.98%
S5	0.09776	212.52%	90.03%
S6	0.09780	212.61%	90.07%

Table 4-3 Carbon dioxide production

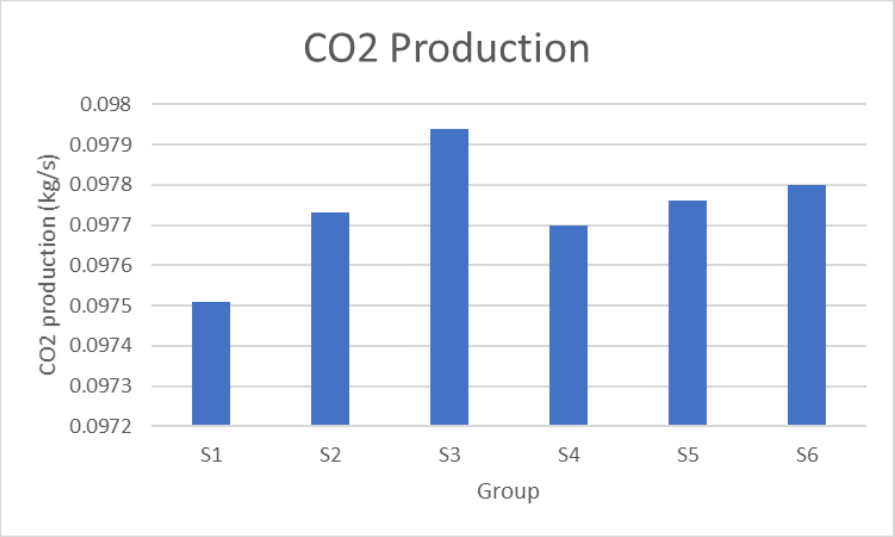


Figure 4-2 CO2 production

As can be seen from **Figure 4-9**, the variation of CO2 production along with UFL change does not follow a certain pattern. This is because when increasing UFL, the CO2 production of the SOFC will increase, while that of the water gas reactions will decrease due to the fact that less CO is being generated from the SOFC at higher UFL. Therefore, by adding up the amount of CO2 production of both, a random trend is witnessed. Besides, the reason why mole percentage is not equal to 100% is that not all the CO is converted by the WGS reactions, a slight amount of CO will enter the tail gas of the Gas Processing System, which can be either combusted or captured.

4.1.2.3 Power output of the SOFC and the PEMFC

The power output of the SOFC and the PEMFC is shown in **Table 4-4**. The Gross Power is acquired by adding them up.

Group	SOFC Power (KW)	PEMFC Power (KW)	Gross Power (KW)
S1	921.2	282.9	1204.1
S2	938.9	253.4	1192.3
S3	955.3	223.3	1178.6
S4	970.5	192.6	1163.1
S5	984.2	162.5	1146.8
S6	996.5	132.5	1129.0

Table 4-4 Power output

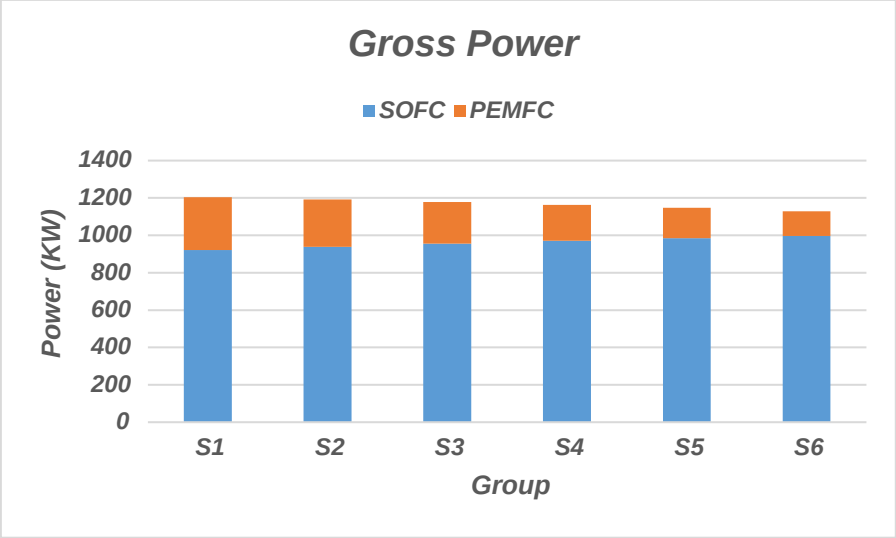


Figure 4-3 Gross Power

With an increasing UFL, the power output of the SOFC is seeing an increasing trend because more fuel is converted into electricity. However, the power output of the PEMFC is seeing a decreasing trend because less hydrogen is produced. When sum up the gross power output of the SOFC and PEMFC, it shows that the gross power output is higher at a lower UFL, which coincides with some previous research. (Fernandes, Woudstra, Wijk, Verhoef, & L. Aravind, 2016)

4.1.2.4 Auxiliary consumption

The auxiliary consumption of each subsystem is shown in **Table 4-5.**

Group	SOFC AUX (KW)	GPS AUX (KW)	PEMFC AUX (KW)	Overall AUX (KW)
S1	73.6	75.2	18.6	167.3
S2	87.9	71.6	16.7	176.2
S3	102.9	68.0	14.8	185.7
S4	117.0	64.2	13.1	194.3
S5	133.2	60.5	11.3	205.0
S6	149.8	56.8	9.5	216.1

Table 4-5 Auxiliary consumption

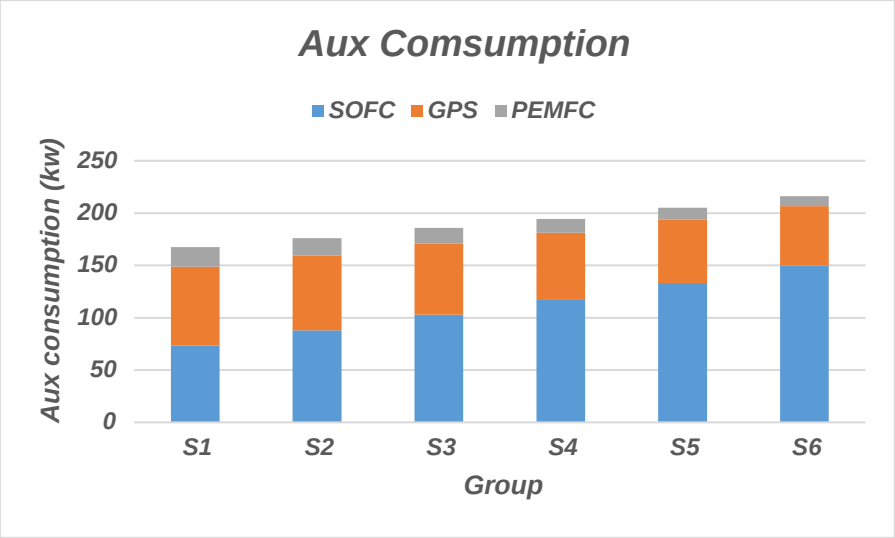


Figure 4-4 Aux Consumption

The overall auxiliary consumption is mainly from the SOFC system and the Gas Processing system. In the SOFC system, the consumption of the air blower contributes the most because a great amount of air is needed to cool the SOFC down. When UFL is higher, more fuel is converted, which means more heat will be generated. Therefore, more power is required from the air blower. For Gas Processing system, the compressor before the PSA system consumes most of the auxiliary power. The pressure requirement of the gas going into the PSA is as high as 2.1MPa. The reason why the auxiliary consumption of the Gas Processing system reduces along with increasing UFL is that less CO will be converted by the WGS reactions in a higher UFL condition. As a result, less gas will enter the PSA system, and hence less power consumption of the compressor before it. The overall auxiliary consumption is seeing an increasing trend, which means the auxiliary consumption in the SOFC system is dominant.

4.1.2.5 Overall power output of the system

By taking into account the auxiliary consumption, the overall power output is given in **Table 4-6.**

Group	SOFC Net Power Output (KW)	PEMFC Net Power Output (KW)	GPS Consumption (KW)	Overall Power Output (KW)
S1	847.7	264.3	75.2	1036.8
S2	851.0	236.7	71.6	1016.1
S3	852.4	208.5	68.0	992.9
S4	853.4	179.6	64.2	968.8
S5	851.1	151.2	60.5	941.8
S6	846.7	123.0	56.8	912.9

Table 4-6 Overall power output

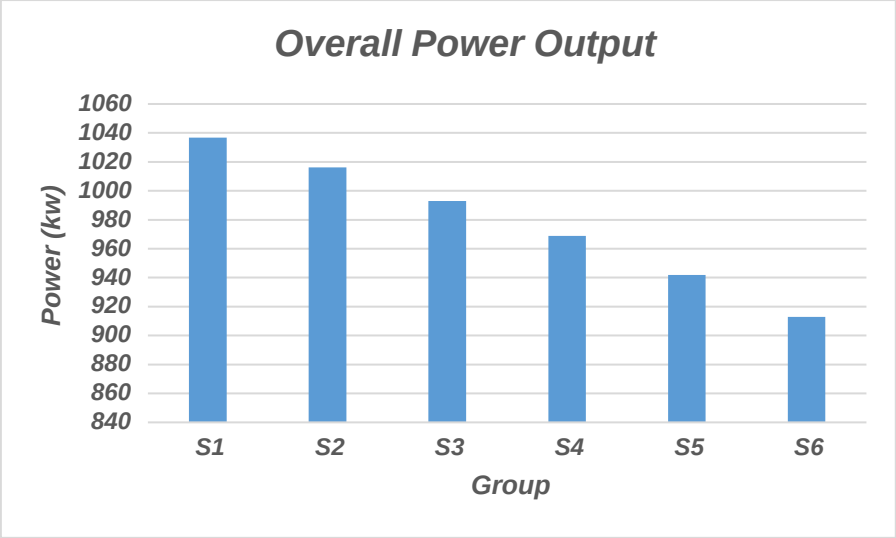


Figure 4-5 Overall Power output

The overall power output still witnesses a decreasing trend after taking the auxiliary consumption into account. It should be mention that the decreasing trend is even sharper than that of the gross power. This means that a tandem fuel cell system may benefit more at a low UFL operational condition.

4.1.2.6 Overall efficiency of the system

The overall efficiency of the system is given in **Table 4-7.** The overall efficiency is calculated by:

$$\frac{overall\ power\ output}{LHV_{NG} \times \Phi_{NG}} \times 100\% \qquad (4.1)$$

Group	Overall Efficiency
S1	59.31%
S2	58.13%
S3	56.80%
S4	55.43%
S5	53.88%
S6	52.22%

Table 4-7 Overall efficiency

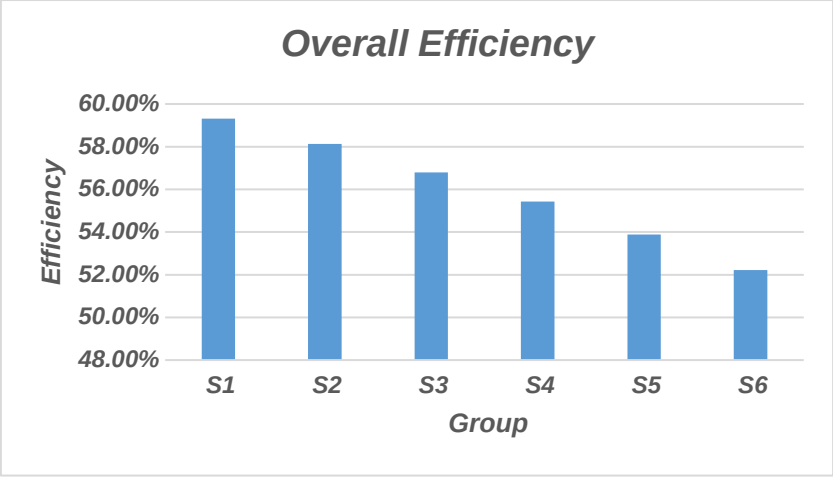


Figure 4-6 Overall efficiency

Again, the trend of overall efficiency shows that at a lower UFL, or higher hydrogen production mode, the efficiency of the whole system is higher. At a high hydrogen production mode, for example S1, the overall efficiency of the whole system can be of the same level as a diesel generator system. This means that more study into this type of system is worthwhile, and it may also imply that this type of system has the potential of partly replacing some of the current existing diesel generator system.

The result of the research paper (Fernandes, Woudstra, Wijk, Verhoef, & L. Aravind, 2016) is shown in **Figure 4-7**.

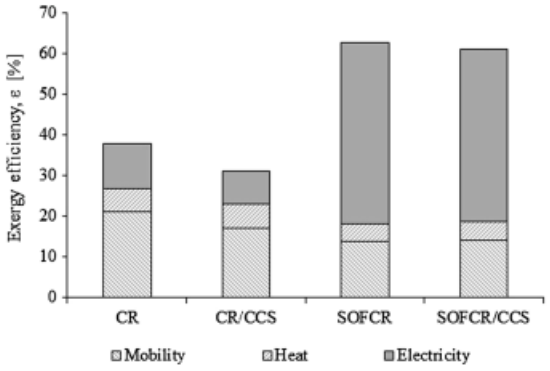


Figure 4-7 Efficiency results of the previous research

In this research, four operation modes are studied. The SOFCR mode and SOFCR/CCS mode are of the same concept as the tandem system. The only difference between the two is whether a carbon capture and storage system is employed. As can be noticed in ***Figure 4-7***, this factor does not make much difference on the results. In both SOFCR and SOFCR/CCS cases, the UFL per pass of the SOFC is set to be around 0.65, which is the same as the setting of S1 of the stationary model. Therefore, the results of them can be compared. ***Figure 4-7*** clearly shows the composition of the overall efficiency. The efficiency components of electricity and heat are straightforward, while the efficiency of mobility needs a little explanation: in this research paper, the tandem fuel cell system is applied in a hydrogen refilling infrastructure site. Apart from being used by PEMFC to generate electric power, the excessive hydrogen is going to be stored for refilling purpose. In other words, this efficiency represents the part of energy being stored in the form of hydrogen. However, in the stationary model of this master thesis, this part does not exist, because it is assumed at the very beginning that all the hydrogen being produced is going to be consumed by the PEMFC. That is to say, the electrical efficiency of the stationary model is the combination of both the efficiency of electricity and mobility as in the research paper. Besides, the efficiency of heat is not taken into account in the stationary study of this master thesis. Therefore, although overall efficiency of the SOFCR and SOFCR/CCS mode are both above 60%, after getting rid of the heat component, the result is close to that of the stationary study (59.31%).

4.2 Simulation 2

4.2.1 Introduction to the simulation

As is mentioned before, this simulation functions as a prelude for the dynamic modeling section. In the tandem fuel cell system, the transient behavior of the SOFC system can hardly meet the requirement of normal operation when transient load condition appears. By employing the PEMFC system, which has a rather satisfactory transient capability, the overall transient capability will be enhanced greatly. In normal operation condition, an operational profile of power requirement that the tandem fuel cell system would come across may be similar to **Figure 4-8**

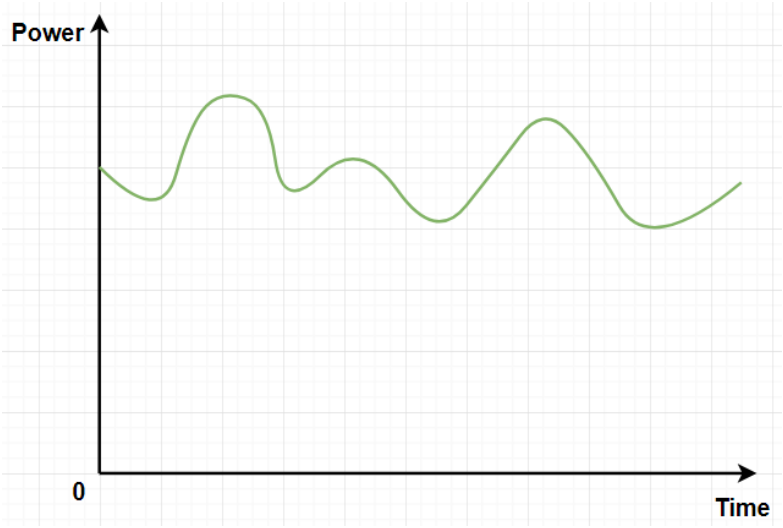


Figure 4-8 Operational profile the system may come across

For the tandem fuel cell system, when coping with this type of transient load condition, the strategy will be: the SOFC system provide the baseline of the power output, while the PEMFC system deal with the transient based on this baseline. The concept of this strategy is illustrated in the **Figure 4-9**.

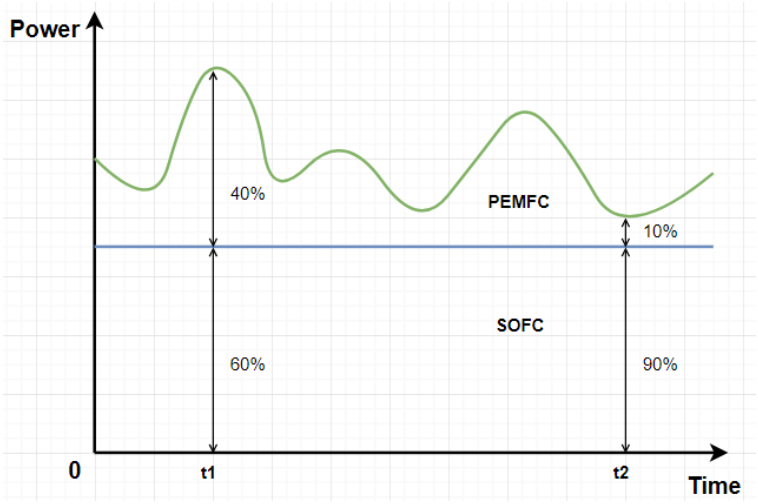


Figure 4-9 Power distribution strategy

As is shown in **Figure 4-9**, when experiencing transient load, the requirement of power output distributed to the SOFC and PEMFC constantly varies along with time. For instance, at time point t_1 , the SOFC is providing 60% of the total power, while the PEMFC is providing 40%. However, at time point t_2 ,90% of the total power is from the SOFC, while PEMFC only contributes to 10%

of the total power output. Because the operational characteristics of SOFC and PEMFC differ a lot from each other, different power distributions may result in different overall performance of the system. Having this in mind, studying the performance of the whole system under different power distributions becomes necessary.

For one certain time point, the power output of the system as well as the power distribution is fixed. Therefore, it can be regarded as a stationary operation condition. For this reason, Cycle-tempo can still be used to study the performance of the system under different power distributions.

4.2.2 Design of the simulation

In this simulation, the variables are the power distributions between the SOFC and the PEMFC. Three sets of power distributions are chosen in this simulation, which are:

Set number	SOFC	PEMFC
1	90%	10%
2	75%	25%
3	60%	40%

Table 4-8 Power distribution (percentage)

Apart from the power distribution, the fuel utilization factor of the SOFC should also be taken into account, because it is a crucial factor that will influence the hydrogen production of the SOFC, thereby, influencing the power output of the PEMFC. Therefore, the simulation will be performed in two groups, with 0.65 (group 1) and 0.85 (group 2) of the SOFC UFL respectively.

In both groups, the overall power output of the whole system is to be set at 1000KW, so the resulting power requirement of the SOFC and the PEMFC will be:

Set number	$P_{SOFC}\ (KW)$	$P_{PEMFC}\ (KW)$
1	900	100
2	750	250
3	600	400

Table 4-9 Power distribution (power)

The setting of the overall power output is realized by setting the power output of the SOFC and PEMFC separately. However, a problem would occur that in one simulation set, the hydrogen produced from the SOFC and gas processing system may not be equal to the hydrogen demand from the PEMFC. In order to deal with this situation, a hydrogen storage system will be employed in the system.

For instance, in simulation (group 2, set 3), the power demand from the PEMFC is quite high while the UFL of the SOFC is also relatively high, which means the instantaneous hydrogen production from the SOFC and gas processing system may not be able to fulfill the requirement of the PEMFC. In this case, the hydrogen storage system will supply the hydrogen deficiency. In simulation (group 1, set 1), however, the instantaneous hydrogen production from the SOFC may be excessive. In this case, the excessive hydrogen will be stored in the hydrogen storage system.

4.2.3 Results and analysis

The simulation results of hydrogen production and demand is shown in **Table 4-10**.The amount of hydrogen from hydrogen storage system is calculated by “Demand minus Production”. When the value is positive, it means that hydrogen is going from the storage system to the PEMFC; while when it is negative, it means the extra hydrogen is going into the storage system.

Group 1			
Set	**Production (kg/s)**	**Demand (kg/s)**	**From storage (kg/s)**
1	0.00410	0.00156	-0.00254
2	0.00325	0.00391	0.00066
3	0.00250	0.00625	0.00375
Group 2			
Set	**Production (kg/s)**	**Demand (kg/s)**	**From storage (kg/s)**
1	0.00151	0.00156	0.00005
2	0.00119	0.00391	0.00272
3	0.00091	0.00625	0.00534

Table 4-10 Hydrogen production and demand

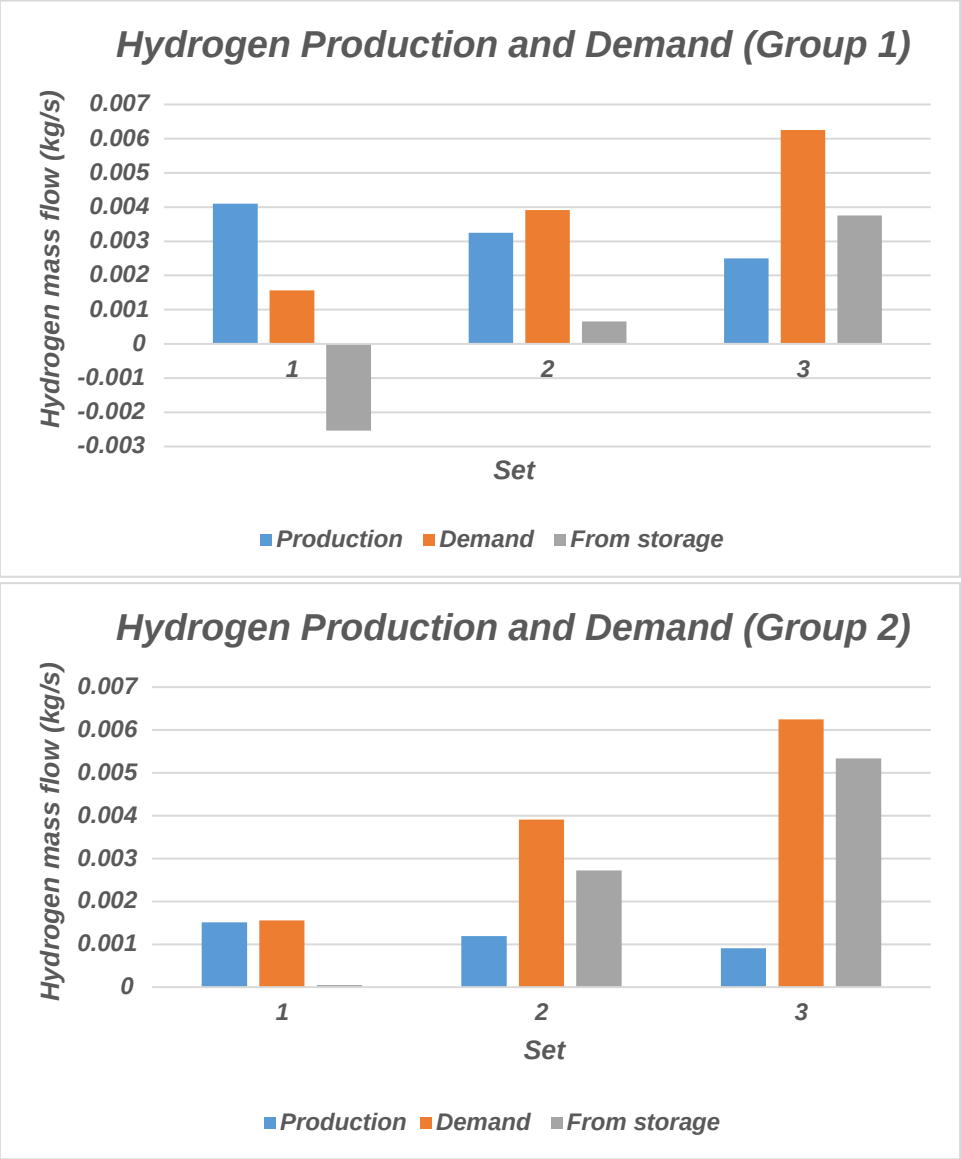


Figure 4-10 Hydrogen production and demand

As can be seen from **Table 4-10**, only in simulation (group1, set 1), hydrogen production exceeds the demand. In the other cases, hydrogen supplement is required from the storage system. In group 1,

the instantaneous hydrogen production meets the demand at the power distribution of around 75%SOFC and 25%PEMFC; while in group 2, this point is reached at around 90%SOFC and 10%PEMFC. It can also be concluded from the result that the load-and-unload capacity of the hydrogen storage system should be at least 0.00534 kg/s in this simulation case.

5. Dynamic model

5.1 Introduction

The second part of this graduation project is to build up a dynamic model of the tandem fuel cell system in Matlab/Simulink. In contrast with the Cycle-tempo model, which is for stationary operation study, this dynamic model will be used to examine the transient behavior of the system.

From this model, a general overview of how the system would response under different demand signals can be acquired. Besides, the capacities of the tanks in the system can be estimated in different scenarios. Both two factors are critical for the design phase. As is stated in **Chapter 1**, besides modeling the tandem fuel cell system, another goal of the study of this master thesis is to develop the prototype of a design tool. This design tool can assist the design phase, in which sizing the tanks and checking the system's transient response are of great concern. The foundation of the design tool is the dynamic model. That how the dynamic model is further developed into the design tool and the relevant details will be described in **Chapter 6**.

To build a desirable dynamic model, two main elements must present:
(1) A transient load as input;
(2) A system model that will dynamically response to the transient load.

The transient load patterns can vary a lot in different situations, especially for ships. The most ideal transient load input would be the one from a real ship operational profile. However, these real-life operational profiles are often limited to be accessed to. Besides, this dynamic model is meant to be an assistance tool for design phase. In this phase, only a rough estimation of the main characteristics is required. Therefore, there is no need to develop this model into a rather detailed one which comprehensively captures all the characteristics of the system. A relatively simple model would be sufficient.

Above all, for this stage, it would be more rational to use several simple transient load patterns as input to test the response of the system, which can provide a general overview of the system's transient behavior. A more comprehensive simulation, with more complex system model and more complex input, can be left for further study.

5.2 Model description

5.2.1 The fuel cell model

The starting point of this study is a fuel cell model which can simulate both PEMFC and SOFC. Thanks to the work of P. de Vos and H. T. Grimmelius (de Vos & Grimmelius, 2009), the author did not need to develop any individual fuel cell models in this study. A detailed description of this model can be found in Appendix.

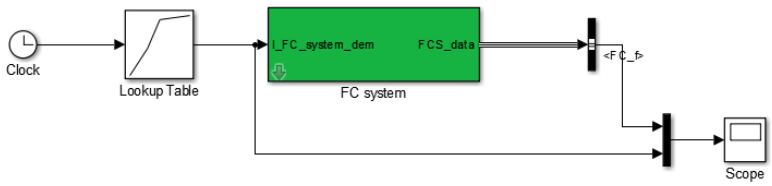


Figure 5-1 General overview of the fuel cell model

5.2.2 Fuel cell characteristics

The polarization curves of SOFC and PEMFC produced by the model are shown in **Figure 5-2.** The voltage/current and power/current curves of SOFC and PEMFC produced by the model are shown in **Figure 5-3.**

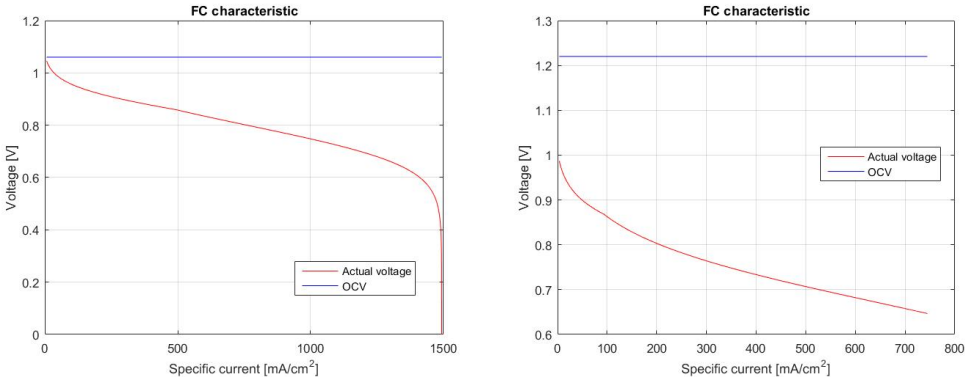


Figure 5-2 Polarization curves of SOFC and PEMFC produced by the model

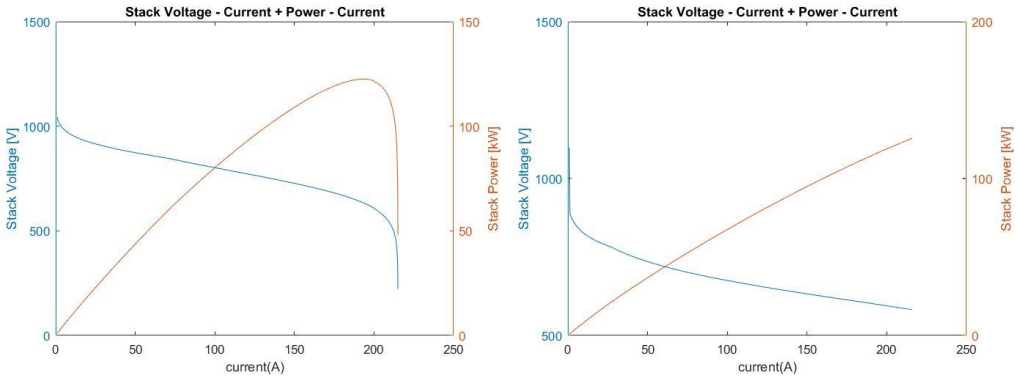


Figure 5-3 Voltage/current and power/current curves of SOFC and PEMFC produced by the model

5.2.3 Anti-causal System

The reader may have already noticed that the input and output of this fuel cell model is reversed when compared to a real fuel cell system whose input is fuel and output is current. In reality, the current of the fuel cell is the result of fuel consumption, which means in time domain, the generation of current happens after the fuel is consumed. However, for this fuel cell model, the generated current

determines the fuel consumption. In other words, something happens in the future determines something happened in the past in this system. This type of system is called “Anti-causal System”.

By definition, an anti-causal system is one that depends on future input values. (Oppenheim, Willsky, & Nawab, 1998)In contrast, a causal system is one whose output depends on past and current inputs. In general, most nature or physical reality is considered to be a causal system. Anti-causal system models are mostly hypothetical or for the convenience of analysis. They are normally used in design studies. For example, when the system is not yet built, an anti-causal model of the system may be developed to assist the design phase, especially in terms of estimate the capacity of the components.

Because the fuel cell model is anti-causal, it is impossible to simulate the real operation of a fuel cell system with it. However, this does not mean the model is useless. As is mentioned above, an anti-causal model is rather useful for design purpose. Besides, since this dynamic model is the very first version, which means a lot of details are absent. From this point of view, an anti-causal model is a better starting point than a causal model, since a less complex modeling process is required while it is still able to reflect the physics of the system to a large extent. After discussing with my supervisor Mr. de Vos about this, we came to an agreement that for current stage, attention should be paid on developing a dynamic model for design purposes, which will be elaborated in **Chapter 5.3**. Further development and supplement (such as developing a causal fuel cell model and applying control theories) can be left for other researchers.

5.2.4 The dynamic tandem FC model

The conceptual layout of this dynamic tandem FC model is shown in **Figure 5-4**

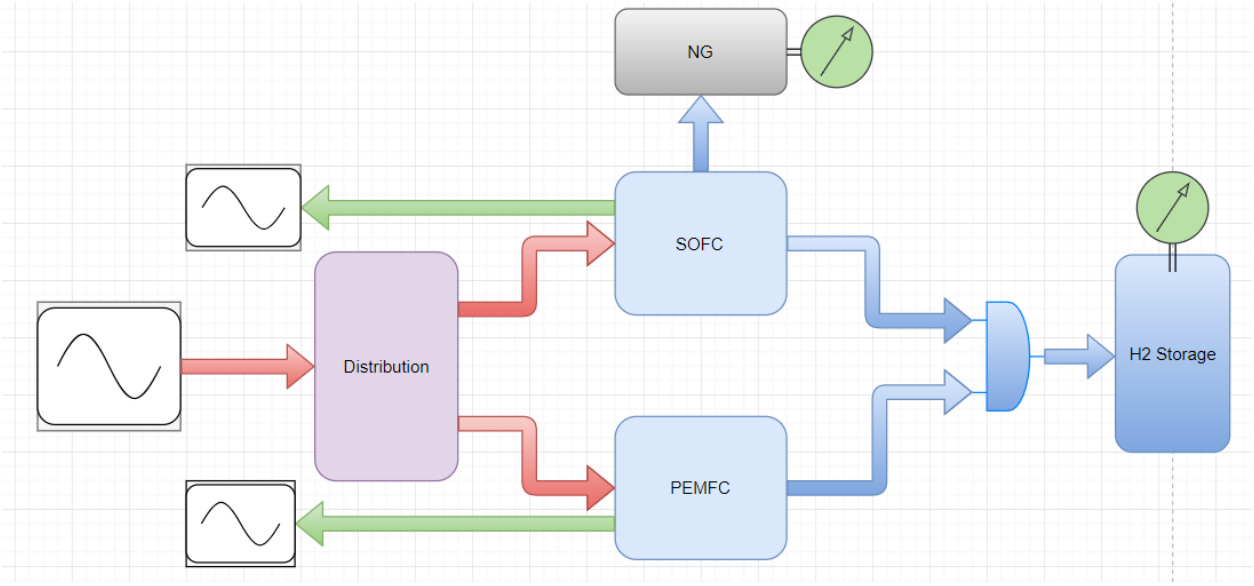


Figure 5-4 Conceptual layout of the dynamic system

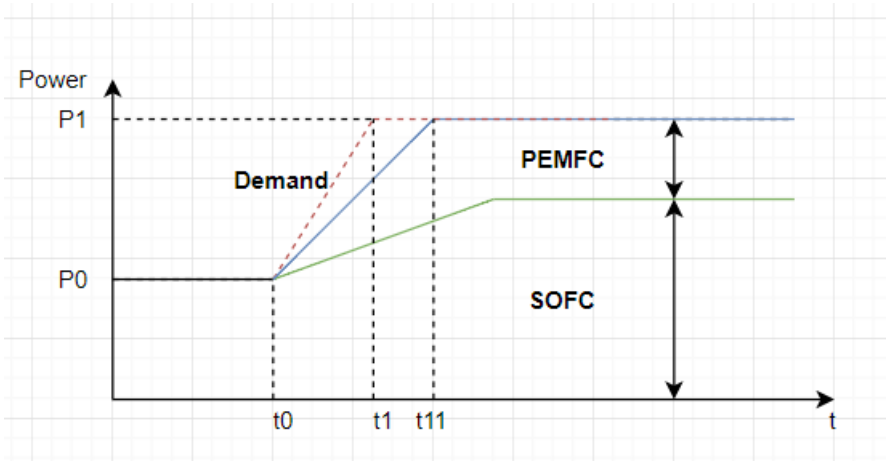
5.2.4.1 power distribution

The dynamic current signal is the input of the system. Since the PEMFC and SOFC will operate together to meet this current demand, a distribution platform, which splits the current into two parts, is required before the fuel cells. Due to the different transient response capabilities of SOFC and PEMFC, the distribution strategy has to be carefully made in order to take fully advantage of both fuel cells. As has been described in the research assignment report, the transient response capability of PEMFC can be close to that of batteries, which is almost instant response. However, that of SOFC is rather

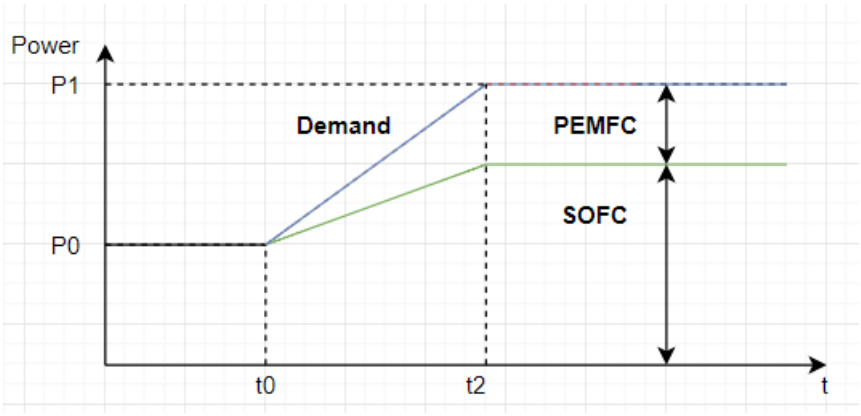
slow, mainly because of the slow mass-transport dynamics. (Sedghisigarchi & Feliachi, 2004) There are plenty of options for the power distribution strategy. However, when considering one of the initial requirements of the system, which is “SOFC to provide the power baseline, while PEMFC to cope with most of the dynamics”, the number of options are restrained. In this model, the power distribution strategy is selected as such that the transient capability of the SOFC is fixed at the maximum, while the PEMFC’s transient capability deals with the left. Here is an example (see **Figure 5-5**)**:**

In case 1 the power demand rises from P0 to P1 in the period of t0 - t1. Because the power demand rises too sharply, although both SOFC and PEMF are running at their highest slew rate, the power demand still cannot be instantly fulfilled. Finally, at t11, the fuel cells reach the output of P1.

In case 2, the power demand still rises from P0 to P1, but in a longer period of t0 - t2. In this case, the slew rate of the SOFC is still at its maximum, but that of PEMFC is not. The slew rate of the SOFC is fully taken advantage of to meet the demand, and the rest will be dealt with by the PEMFC.



Case 1

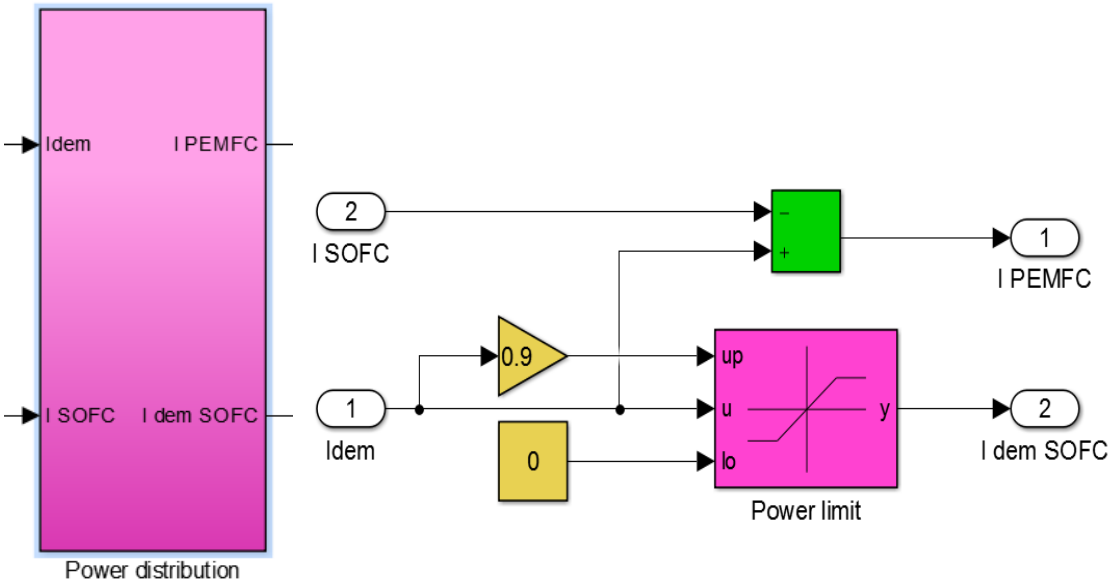


Case 2

Figure 5-5 Power distribution example

As can be noticed in case 1 of the example above, the power output of the SOFC still rises even after the system has already meet the power demand. This is because for stationary operation, in order to reduce the consumption of hydrogen, the output of the PEMFC should be limited. As a result, the ratio between the power output of SOFC and PEMFC will be set at a specific value where hydrogen consumption is not too high.

The diagram of the distribution platform in Simulink is shown in **Figure 5-6**:



(a) Overall view (b) Detailed view

Figure 5-6 Power distribution block

As can be seen in the overall view of the "Power distribution" block, the inputs are "I dem" (current demand) and "I SOFC" (current supply of the SOFC), and the outputs are the current demand for SOFC and PEMFC. Why the current supply of the SOFC is needed in power distribution can be explained by describing the details of the block. The current demand of the PEMCF is equal to the total power demand minus the current supply of the SOFC. That is:

$$I_{dem\ SOFC} = I_{dem\ tot} - I_{sup\ SOFC} \qquad (5.1)$$

There are two possible relations between the slew rate of $I_{dem\ tot}$ and the maximum slew rate of $I_{sup\ SOFC}$, namely $\frac{d}{dt}I_{dem\ tot} \leq \frac{d}{dt}I_{sup\ SOFC}$ or $\frac{d}{dt}I_{dem\ tot} > \frac{d}{dt}I_{sup\ SOFC}$. If $\frac{d}{dt}I_{dem\ tot} \leq \frac{d}{dt}I_{sup\ SOFC}$, SOFC can meet the requirement by itself without the assistance from the PEMFC. Therefore, $I_{dem\ tot}$ will be equal to $I_{sup\ SOFC}$ all the time, which means $I_{dem\ PEMFC}$ will be 0. If $\frac{d}{dt}I_{dem\ tot} > \frac{d}{dt}I_{sup\ SOFC}$, SOFC will not be able to fulfill the demand. In this case, the SOFC will operate at its highest slew rate, and the deficiency between the current demand and the SOFC output current will become the input of the PEMFC. In both cases, the SOFC's slew rate are fully taken advantage of.

The "power limit" block is to limit the power output ratio between the SOFC and the PEMFC when stationary operation, which has already been explained.

As is mentioned above, the main consideration of this strategy is to take fully advantage of the transient of the SOFC. When taking other considerations in to account, there might be more optimal solutions. However, this is not within the scope of this study. Attention can be paid here for further research.

5.2.4.2 NG consumption

One of the main purposes of this dynamic model is to determine the capacity of the fuel tank based on the operational profile, in other words, to determine how much NG is going to be consumed for a given scenario.

The original SOFC model is capable of calculating the fuel consumption, but the fuel is hydrogen. Since NG is the fuel in the tandem fuel cell system, the fuel consumption of hydrogen has to be converted into that of NG. Although NG is a mixture, more than 97% (mole fraction) of it is CH_4. There are also other hydrocarbons that can be consumed by the SOFC, but only make up less than 2%. Therefore, for the convenience of calculation, it is assumed that NG is pure CH_4.The relation between hydrogen consumption and NG consumption is:

$$\dot{m}_{CH_4} = \frac{\dot{m}_{H_2}}{4 \cdot UFL_{SOFC}} \tag{5.2}$$

And the capacity of the NG tank is:

$$m_{CH_4\,tank} = \int_0^{t_{end}} \dot{m}_{CH_4}(t)\,dt \tag{5.3}$$

Where,

$\dot{m}_{CH_4}$ is NG consumption (kg/s);

$\dot{m}_{H_2}$ is hydrogen consumption (kg/s);

UFL_{SOFC} is the fuel utilization factor of the SOFC. According to the results of the stationary model, it is set to be 0.65 here (-);

$m_{CH_4\,tank}$ is the capacity of the NG storage tank (kg);

t_{end} is the time at which operation (simulation) ends (s).

5.2.4.3 H2 storage

The hydrogen storage system, which is also a crucial part in the system, is also going to be sized in this dynamic model. Apart from time, there are two variables influence the sizing: the instantaneous hydrogen consumption of the PEMFC, and the instantaneous hydrogen production of the SOFC. The relation between the capacity and these variables is:

$$m_{H_2\,tank} = \int_0^{t_{end}} (\dot{m}_{comsume}(t) - \dot{m}_{produce}(t))\,dt \tag{5.4}$$

$m_{H_2\,tank}$ is the volume of the hydrogen storage tank (kg);

$\dot{m}_{comsume}$ is the instantaneous hydrogen consumption of the PEMFC (kg/s);

$\dot{m}_{produce}$ is the instantaneous hydrogen production of the SOFC (kg/s);

t_{end} is the time at which operation (simulation) ends (s).

6. Dynamic model simulation

According to the study goal of this dynamic model, the transient response of the system is going to be examined by simulation. Furthermore, the capacity of both the fuel tank and the hydrogen storage tank are going to be estimated. Four typical power demand signals will be the tested, namely, step signal, sinusoidal signal, impulse signal and random signal. The simulation time is fixed to be 300s.

In order to be align with the stationary simulation in Cycle-tempo, the rated power of the SOFC and PEMFC are set to be 600 KW and 400KW respectively. Because the rated power of both SOFC and PEMFC in the given model are around 120 KW, the fuel cell rated power needs to be scaled up. There are two ways to scale up the rated power: scale up the voltage (increasing the number of cells) or scale up the current (increasing the area of single cell). In practice, changing the voltage can bring extra problem to the inverter which transforms the DC from the fuel cell into AC. The AC voltage in the bus is normally fixed, and the fuel cell voltage is designed to be equivalent to the AC voltage. In this way, no transformer will be needed to adjust the amplitude of the voltage. Therefore, only scaling up the current without changing the voltage would be more convenient. In this study, the power output is also scaled up by scaling up the current (increasing the area of single cell). It should also be mention that by increasing the area of single cells, the transient capacity of the fuel cell will also increase proportionally. The relevant data of the given model and the scaled-model is shown **Table 6-1 Fuel cell scaled-up data**.

	GIVEN MODEL		**SCALED-UP MODEL**	
	SOFC	PEMFC	SOFC	PEMFC
$A_{cell}\ (m^2)$	0.0144	0.029	0.72	0.097
N_{cell}	984	900	984	900
$I_{rate}\ (A/s)$	0.653	15.85	3.265	52.83
$P_{cell}\ (kW)$	120	120	600	400

Table 6-1 Fuel cell scaled-up data

6.1 Step signal

In this simulation, a step signal with a step value of 400kw is the input of the system. The response of the system is shown in the **Figure 6-1**.

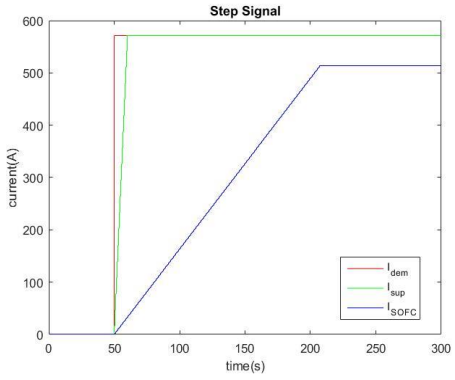


Figure 6-1 Step signal response

As is shown in **Figure 6-1**, although the slew rate of the SOFC is rather slow, the overall response

speed of the system is relatively fast, due to the presence of the PEMFC. The system can fulfill the step current change demand within 10s. The rated power of the whole system is around 1000KW. Therefore, the power increasing rate is:

$$\frac{400/1000}{10} \times 100\% = 4\%/s$$

According to the results in the research assignment, the power increase rate of a diesel engine system is normally within the range of $1.7\,\%/s - 2.5\%/s$. Therefore, it can be concluded that the tandem fuel cell system has a better transient response in terms of power increasing rate.

The hydrogen consumption is shown in **Figure 6-2**.

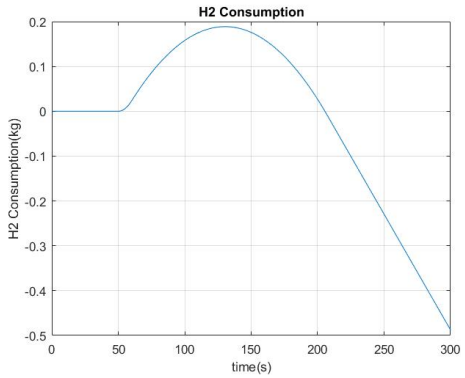


Figure 6-2 Hydrogen consumption

Before 130s, the hydrogen demand of the PEMFC is higher than the hydrogen production of the SOFC, so the whole system is consuming hydrogen during this period. About 0.19kg hydrogen is required from the hydrogen storage tank. After 130s, the hydrogen production becomes higher than consumption. At 205s, the system started to accumulate hydrogen. At the end of the operation, the hydrogen storage tank accumulates 0.48kg hydrogen.

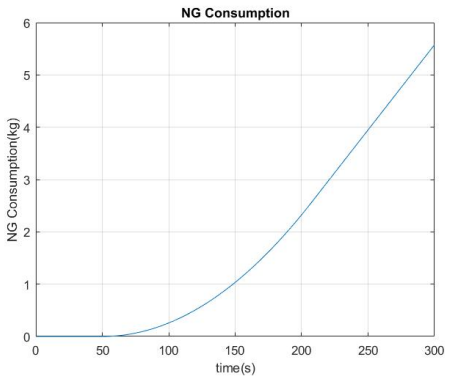


Figure 6-3 NG consumption

The overall NG consumption in this simulation is 5.5kg.

6.2 Sinusoidal signal

In this simulation, a sinusoidal signal, with amplitude of 50kW, period of 1rad/s, and bias of 250kw, is the input. See **Figure 6-4**.

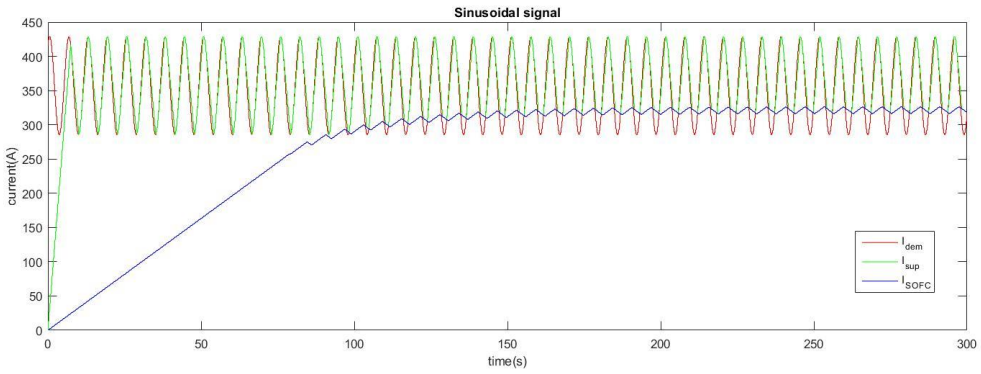


Figure 6-4 Sinusoidal signal response

From **Figure 6-4**, the system can still reach the current demand rather rapidly (within 10s). When the output of the SOFC reaches 90% of the demand, its operation becomes almost stationary due to the low slew rate. The PEMFC, in this case, deals with most of the transients.
The hydrogen consumption is shown in **Figure 6-5**.

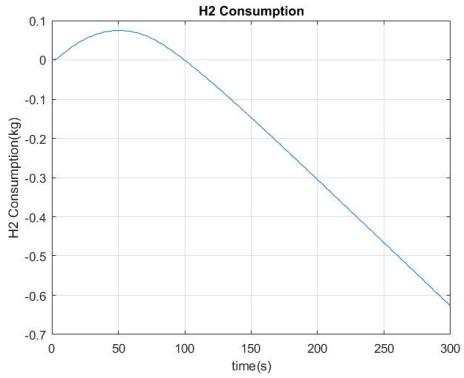


Figure 6-5 Hydrogen consumption

The hydrogen demand has always been higher than production until 50s. About 0.8kg hydrogen is needed to cover the hydrogen consumption of this period. After 50s, hydrogen production becomes higher than demand. In the end, the hydrogen storage tank accumulates 0.62kg hydrogen.

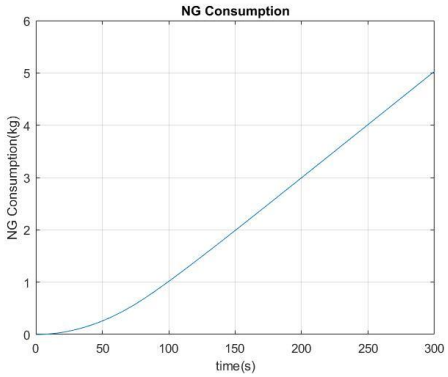


Figure 6-6 NG consumption

The overall NG consumption in this simulation is 5kg.

6.3 Pulse signal

In this simulation, a pulse signal, with amplitude of 100kW, period of 0.1/s, is the input. See **Figure**

6-7.

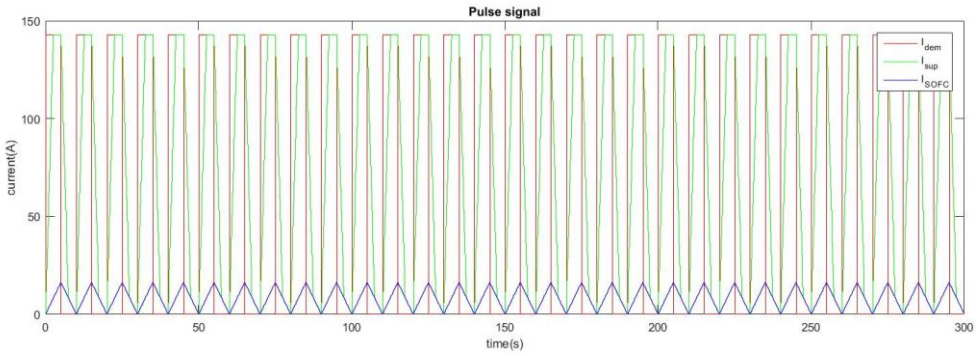


Figure 6-7 Pulse signal response

It can be noticed that when the current demand instantly increases from zero to the pulse value, the system can response rapidly with its highest slew rate. However, when the demand decreases from the pulse value to zero, the slew rate of the whole system will be limited by the SOFC, which renders the output of the system hardly reach zero. This reflects one of the shortcomings of the selected power distribution strategy. When the current demand increase, the system can take full advantage of the slew rate of both fuel cells. However, when the current demand decreases, especially a sharp decrease, the response speed of the system will be limited by SOFC. The higher the output of the SOFC is, the more serious this problem will be. Therefore, when the system is expected to experience sharp decreases in power demand during operation, it is necessary to modify this power distribution strategy or switch into a new one.

The hydrogen consumption is shown in **Figure 6-8**.

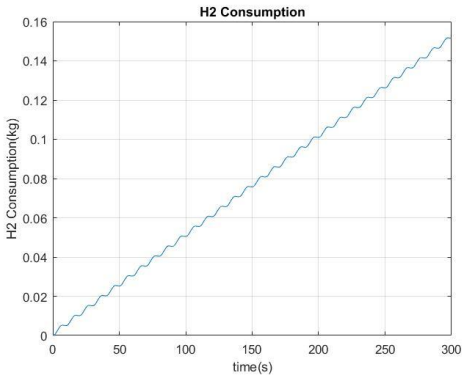


Figure 6-8 Hydrogen consumption

Throughout the whole operation, the SOFC can hardly produce any hydrogen because it is constantly operating at a low power output range. A large amount of hydrogen is required from the PEMFC to meet the transient demand. 0.15kg hydrogen should be stored in the hydrogen storage tank before the operation.

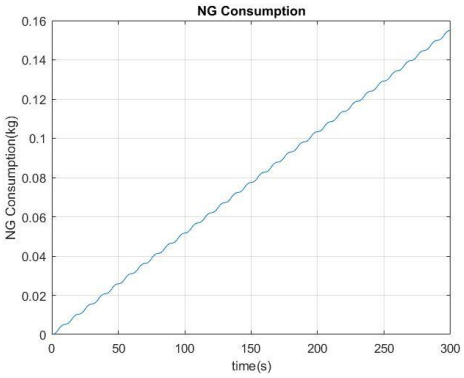


Figure 6-9 NG consumption

The overall NG consumption in this simulation is 0.155kg.

6.4 Random signal

A random signal, with mean value of 200kW and variance of 3×10^7, is fed into the system. The response of the system is shown **Figure 6-10**.

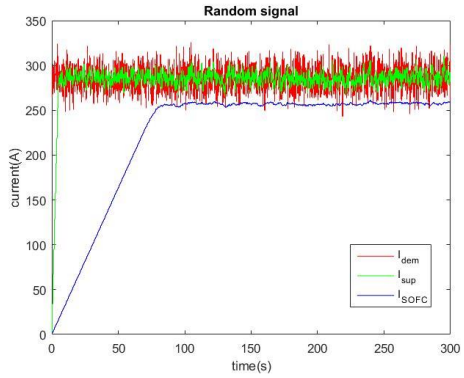


Figure 6-10 Random signal response

From an overall view, it can be said that the system can still fulfill the demand acceptably, except in some cases the current demand increases or decreases too sharply. Again, the abovementioned problem of this power distribution strategy appears in this simulation: when the current demand decreases too sharply, the transient response of the system will be limited by the SOFC. Different from the “pulse signal” simulation, the current demand never decreases to zero. Therefore, a simple modification of the power distribution strategy is to decrease the proportion of the SOFC power output in the total power output. For example, in this case, if it can decrease from 90% to 80%, most of the decreasing transient can be dealt with.

This may bring up a new topic that an accurate prediction of the power demand of the system is rather necessary for determining the power distribution strategy. Experience and big data analysis may be required in this topic. Although this is not in the scope of this study, to assist making an optimal power distribution strategy, attention should be paid on this topic for future researchers.

The hydrogen consumption is shown in **Figure 6-11**.

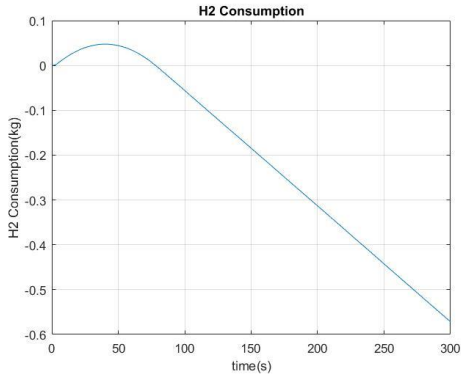


Figure 6-11 Hydrogen consumption

Before 40s, the hydrogen demand is higher than production. About 0.04kg hydrogen is needed from the storage tank in this period. After 80s, the system starts to accumulate hydrogen. In the end, 0.57kg hydrogen is accumulated in the storage tank.

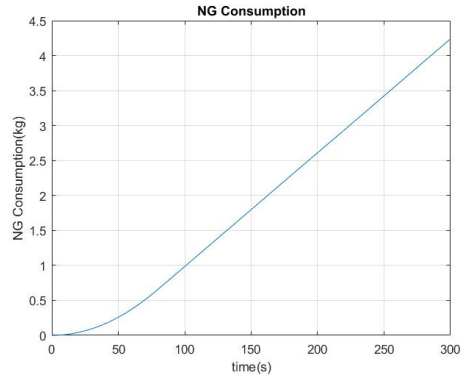


Figure 6-12 NG consumption

The overall NG consumption in this simulation is 4.25kg.

7. Design tool

7.1 Introduction

From the overview of the project (**Error! Reference source not found.**) listed in **Chapter 1**, it can be noticed that the task of developing and updating the design tool is throughout the whole project. In engineering field, computer assistance design has already become a trend, since it can make the design phase much more convenient and efficient, especially when there is a customized design tool for a certain type of system. By using this kind of customized design tool, the designer does not need to rebuild the system model and redo the calculations every time when a new system of the same category is to be designed. Only by inputting the data of requirement, the design tool can output the results of concern. This is the type of design tool that is going to be developed here in this project ─ a customized design tool for the tandem fuel cell system.

In this master thesis, an initial version of the design tool is going be developed. In this version, the design tool should be able to show the transient response of the system under different demand signal. Furthermore, the capacity of the fuel tank and the hydrogen storage tank can be determined according to demand signal and operational time. Other detailed function will be introduced later in this chapter. Since this master thesis is the very beginning of the project and the study of the system is not thorough yet, the accuracy of the results provided by this version of the design tool might not be quite high. However, more important than providing accurate results, this initial version should be perceived as a foundation for the whole process of developing the design assistance tool. It provides the concept and structure of how the design tool should be like. When more knowledge is acquired, more functions and more accuracy will be added in later versions. But no matter how far the later versions go, it is this this initial version that guide the route.

As is stated in Chapter 5, this first version design tool is developed from the dynamic model in Matlab/Simulink. Therefore, for convenience, the design tool is also developed in Matlab platform.

7.2 Tool description

The structure of the design tool is shown in **Figure 7-1**.

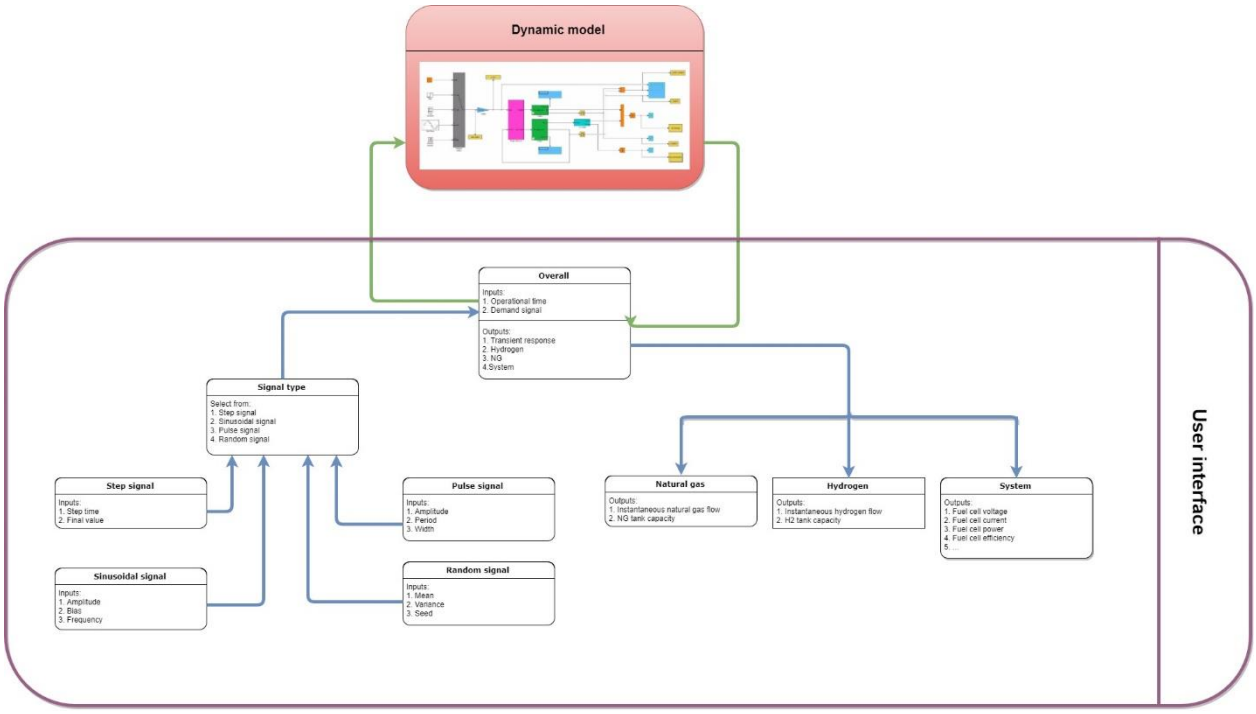


Figure 7-1 Design tool structure

There are two main parts of the tool: the dynamic model and the user interface. Information will be exchanged between each other when the tool works. To use the design tool, the user should firstly specify the operational time and demand signal. The operational time can be specified in the “Overall” window. [see figure]

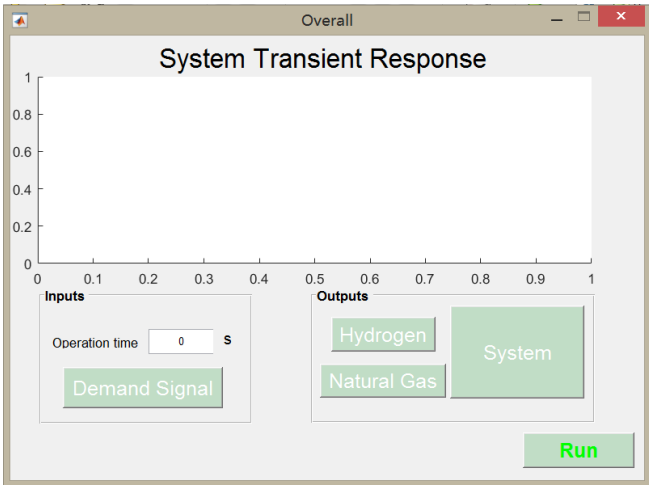


Figure 7-2 Overall window

The demand signal can be specified by clicking the “demand signal” button. After that, a “signal type” window will pop **Figure 7-3**, where the user can choose the type of the demand signal. Currently, there are 4 types of signal available, which are Step signal, Sinusoidal signal, Pulse signal and Random signal. For each type, the details of the selected signal will be asked specifying. (**Figure 7-4**)

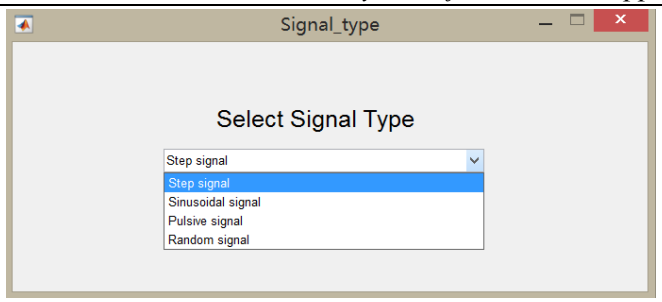


Figure 7-3 Signal type

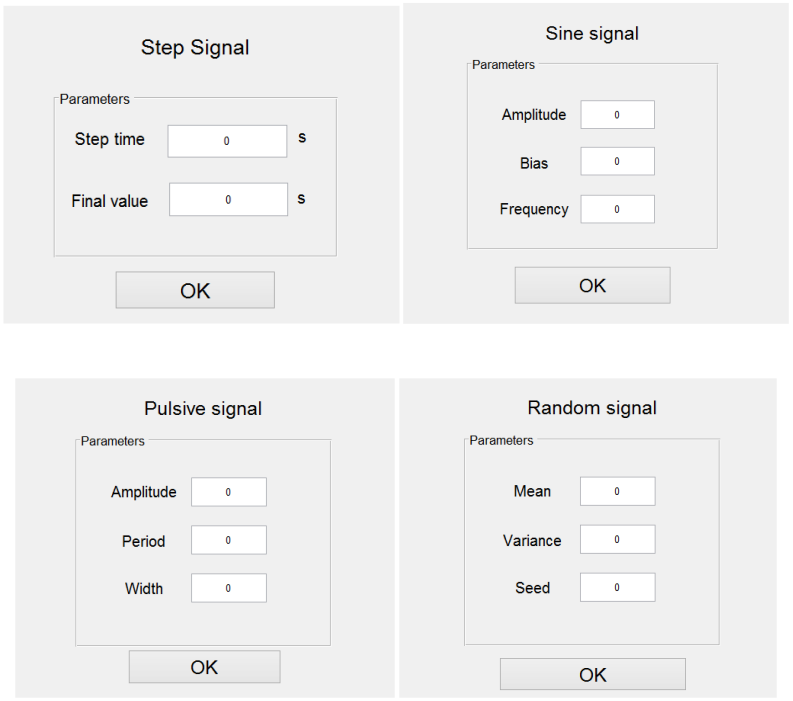


Figure 7-4 Signal specifications

After specifying the inputs, by clicking the run button on the “overall” window, the inputs will be loaded as parameters into the dynamic model, and it will run simulation based on the input parameters and provide results accordingly. The results will then be sent back to the user interface. The transient response will directly be shown on “overall” window. For the results of natural gas tank capacity and hydrogen tank capacity, the user can check them by clicking the buttons on the “output” section of the “overall” window. They will be shown on the corresponding popup windows. (**Figure 7-5**)

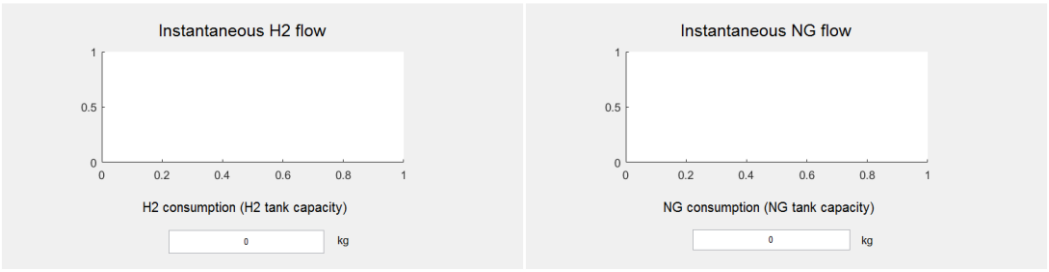


Figure 7-5 Hydrogen and Natural gas

From the description above, it can be seen that the initial version of the design tool is able to fulfill the basic requirement of visualizing the transient response and sizing the tanks. To make the tool more reliable and user-friendly, improvement should be constantly made on both the dynamic model and

the user interface. This should be performed throughout the whole project once the study of the system moves one step further.

8. Conclusion

In **Chapter 1**, the research questions this thesis addresses were formulated. In this chapter, these research questions are going to be repeated and answered.

Research question 1:

Can the efficiency of more than 60% of the tandem fuel cell system as reported in previous research be re-produced?

Answer:

Yes. The result of Simulation 1 in **Chapter 4** shows that when the overall UFL of the SOFC is at 0.8, the overall efficiency of the system can reach 59.31%, which is a desirable reproduction of previous research.

Research question 2:

Is the transient behavior of the system good enough to be equivalent to or even outperform the marine LNG engine power plants?

Answer:

Yes. The power increasing rate of this system can reach $4\%/s$, which is higher than that recommended for marine LNG engine systems. Furthermore, it is also found in the dynamic model that the transient performance of the system and the size of the tanks can be influenced by the power distribution strategy between the SOFC and the PEMFC. For the selected power distribution strategy, the transient behavior of the system is generally acceptable. The power distribution between the SOFC and PEMFC at which the overall hydrogen production equals to zero is around 75% SOFC and 25% PEMFC (3:1).

Research question 3:

How can the design assistant tool help in the design phase of the system?

Answer:

- The design tool can show the system's transient response to different power demand signal, which provides the designer with a general overview of the system's transient behavior in given the scenario.
- The design tool is able to determine the capacity of the fuel tank and the hydrogen storage tank according to the power demand.
- The design enables multiple power distribution strategy to be tested in the system, so the designer can find the optimal one in the given scenario.
- A GUI is created in the design tool, which enables the designer to set input and acquire output without opening the dynamic model manually.

The main research question:

Is the tandem fuel cell system a viable alternative to marine LNG engine power plants?

Answer:

For current stage, this question cannot be totally answered. However, from the answers of research question 1 to 3, it can be concluded that the tandem fuel cell system demonstrates great potential to be an alternative of marine LNG engine power plants theoretically. The contributions this research has made are:

- On the basis of previous researches of the system, the high efficiency has been reproduced in this research.
- Furthermore, the research on the transient behavior of the tandem fuel cell is performed, which has not been done before according to the published literatures. The result turned out that the transient behavior of tandem fuel cell system is higher than that of marine LNG engines theoretically.
- Besides, a primary design tool of tandem fuel cell systems is built in this research. No matter for later research or for the commercialization of the system, this primary design tool will bring convenience in the design phase and set a foundation for the development of a more comprehensive design tool.

So far, it is still unpredictable that how far this project will go. But the results of this master thesis show that it is worthwhile to move forward to the next step. With more effort put into the project, the answer of this main research question will finally be found.

9. Recommendations

(1) The modeling of the PSA section in the stationary model is relatively simple. The power consumption is assumed to be equal to that of a compressor. However, the working mechanism of a PSA system is more sophisticated than a steadily operating compressor, which might result in a more complex power consumption pattern. Since the PSA system makes an essential contribution to the auxiliary consumption, to increase the fidelity of the model, further improvement of its modeling is necessary.

(2) The water management strategy of the tandem fuel cell system still has a great potential to be improved. In the stationary model, the high temperature steam being produced in the gas processing system has not been taken advantage of. To further increase the overall efficiency of the system, investigation into the recycling of this steam is necessary.

(3) The transient response of the system is overly simplified. The only representation of fuel cell dynamics is the “rate limiter” block. It reflects the transient response of the fuel cell to a certain extent. However, there is still a large space for improvement. More transient characteristics should be taken into consideration to increase the fidelity of the model. This can be achieved by applying more detailed fuel cell transient response equations in the model, or directly acquire experiment data.

(4) As is mentioned before, the anti-causal fuel cell model makes it impossible to control the power output by controlling the fuel input, which is a bit counter-intuitive. A causal model should be developed in future research to pave the way for more complex control systems.

(5) The auxiliary components in this dynamic model are only two compressors. However, as can be seen in the stationary model, there are many other auxiliary components presenting in the system, especially in the Gas Processing System. Most of them have influence on the efficiency of the whole system. Therefore, these components should be gradually added into the model in future research.

(6) The control system should take more factors into consideration, such as cold start-up of the SOFC. Besides, a more intellectual power distribution platform should be developed to achieve a better transient performance.

(7) The design tool developed in this study is only a primary version. With the project going further, the design tool should be gradually updated and should be made more functional and user friendly.

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Appendix

1. Transient response of different sinusoidal inputs

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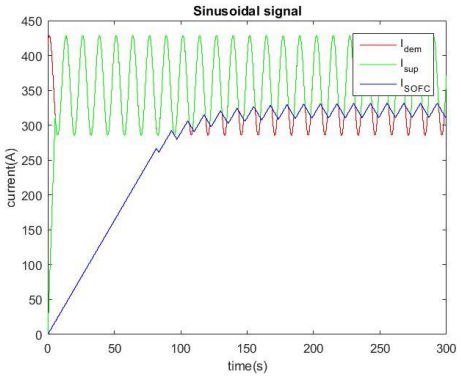

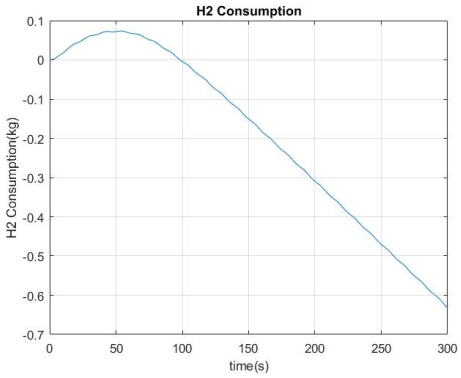

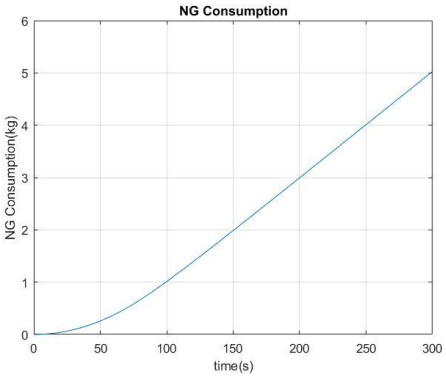

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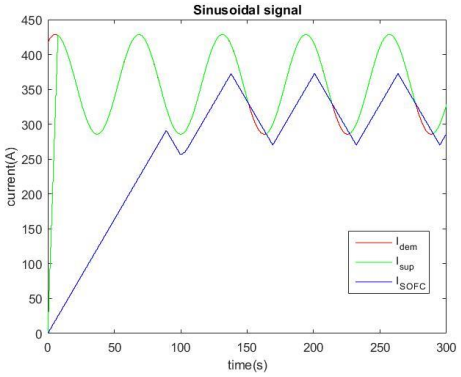
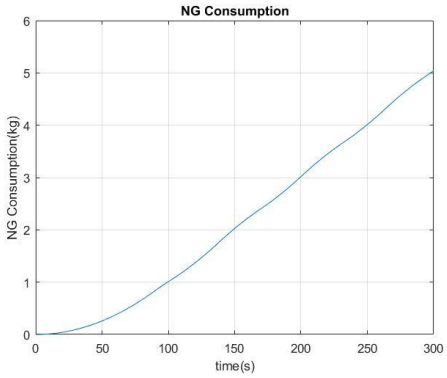
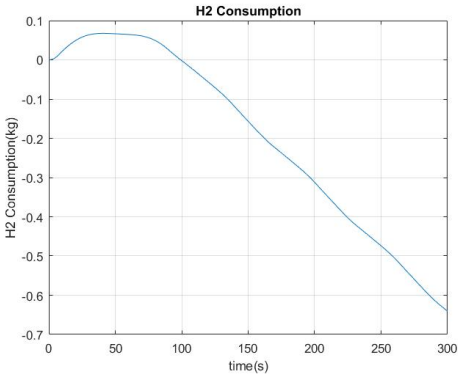
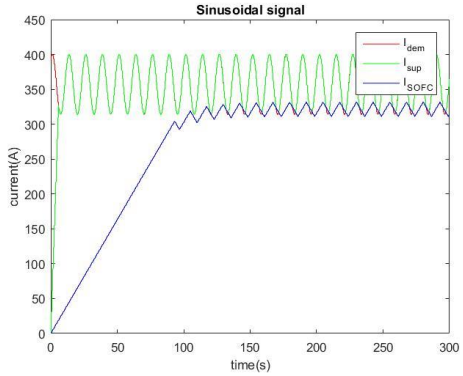
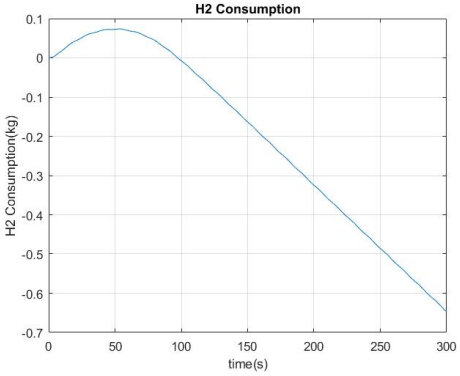


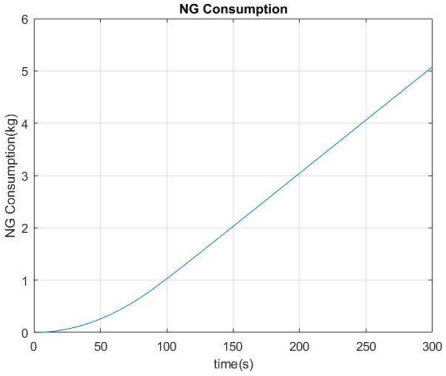




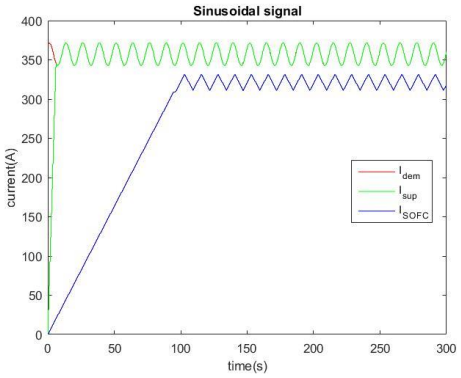
3 rad=0.5, amp=30KW

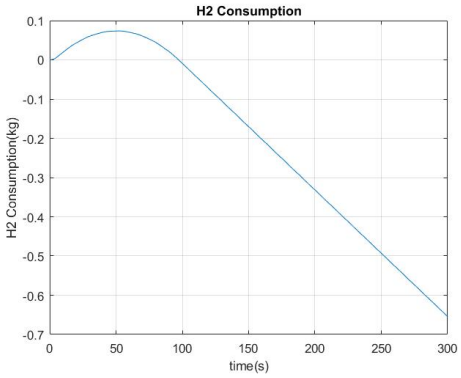


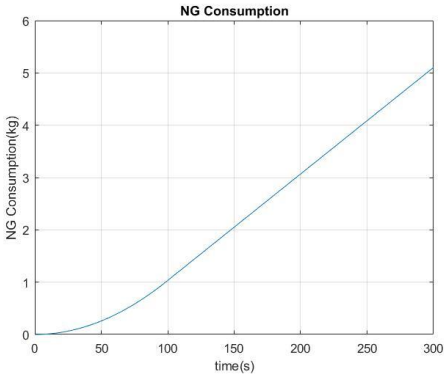




4 rad=0.5, amp=10KW




H2 Consumption
H2 Consumption(kg)
time(s)
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
0
50
100
150
200
250
300


NG Consumption
NG Consumption(kg)
time(s)
6
5
4
3
2
1
0
0
50
100
150
200
250
300

2. Fuel cell model description

LEVEL 1

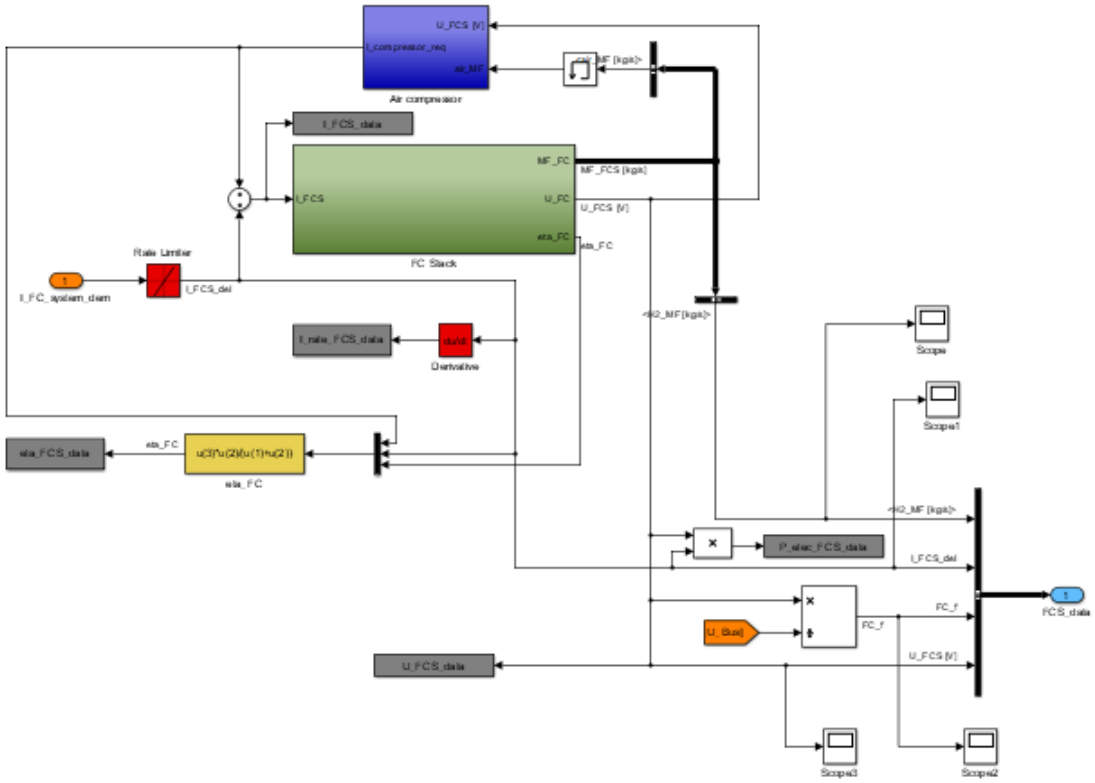
The fuel cell model is relatively simple and straightforward. As is shown in **FC system layout**, the input of the FC system is the time varying current signal, which can be acquired from the operational profile. The FC system block can calculate the operational characteristics (which is designated as FCS_data in the model) of the fuel cell, such as fuel requirement, stack voltage, power output, etc.

The type of the fuel cell can be specified. Three types of fuel cells, namely SOFC, PEMFC and MCFC are available. In this study, SOFC and PEMFC are to be used.

It should be mention that when selecting different types of fuel cells, the system layout within the “FC system” block will not change. What changes is the parameters of the fuel cells, which will lead to different operational profiles. All the parameters of each type of fuel cell are loaded into workspace through a Matlab code “get_parameters”.

LEVEL 2

The system layout within the “FC system” is shown in **FC system layout**.



FC system layout

The two main components are “FC Stack” and “Air compressor”. The “FC Stack” block calculates the abovementioned characteristics based on the input current signal, which is the combination of the current signal from the operational profile and the current requirement of the air compressor. The current requirement of the air compressor is calculated in the “Air compressor” block based on the fuel cell stack voltage and the air mass flow, both of which are outputs of the “FC Stack” block.

Another crucial part in this level is the current rate limiter, which is located directly after the input

demand signal. Although it is only a simple "slew rate" block, the dynamic of the fuel cell is totally represented by it. In a real fuel cell system, if the demand signal changes overly sharply, the fuel cell may not be able to immediately deliver enough current to fulfill the demand. The rate of how fast the delivered current can change (increase or decrease) is limited by the transient capacity of the fuel cells. The "slew rate" block here in this model is to simulate this capacity. It should be mention that the real physical transient response of fuel cells is more complex that of a "slew rate". However, when the fuel cells are manufactured, the manufacturers usually place a rate limiter ahead of the stack to prevent the current from increasing too sharply, causing damage to the fuel cell. Therefore, when testing a real fuel cell system, the transient response would also be similar to a "slew rate" block. Therefore, from a system engineering point of view, since a rate limiter will always present, there is no need to model the real physics of a fuel cell. A "slew rate" block can, to a large extent, reflect the real fuel cell system's dynamic.

The transient capacity of fuel cells can vary a lot from type to type. Therefore, the data in the "slew rate" block are different in the SOFC model and the PEMFC model. Because the "slew rate" represents a limitation of a fuel cell system, the manufacturers normally would not like to publish its value. When the fuel cell model was initially developed, this data was acquired from industry insiders. Although the data from the manufacturers can be hardly accessed to, a general estimation can be found from literature. See **SOFC power slew rate**.

Power slew rate ($W\ s^{-1}$)	Maximum ΔT derivative ($K\ s^{-1}$), $\Delta T = T_{out} - T_{in}$
Inf	635
800	50
400	23.5
80	4.75
8	0.5

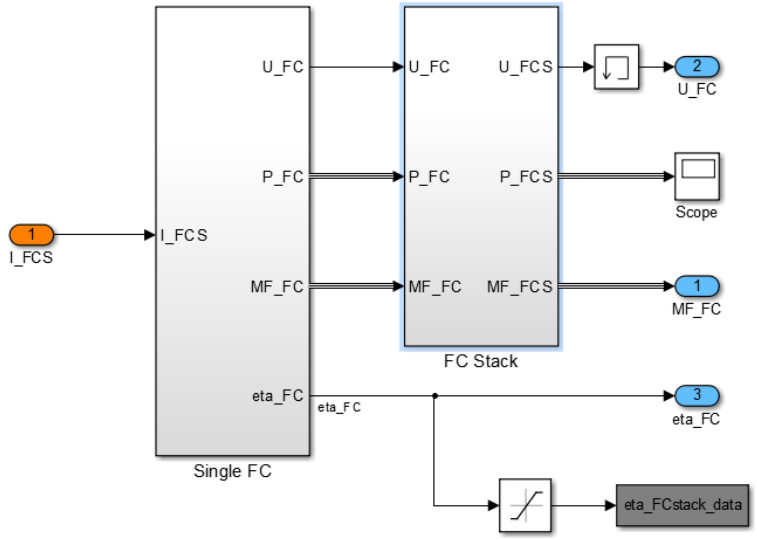
SOFC power slew rate (*(Dario Marra, 2016)****)***

In the given model, the power slew rate of the SOFC is around 450 W/s, which is a reasonable value.

LEVEL 3

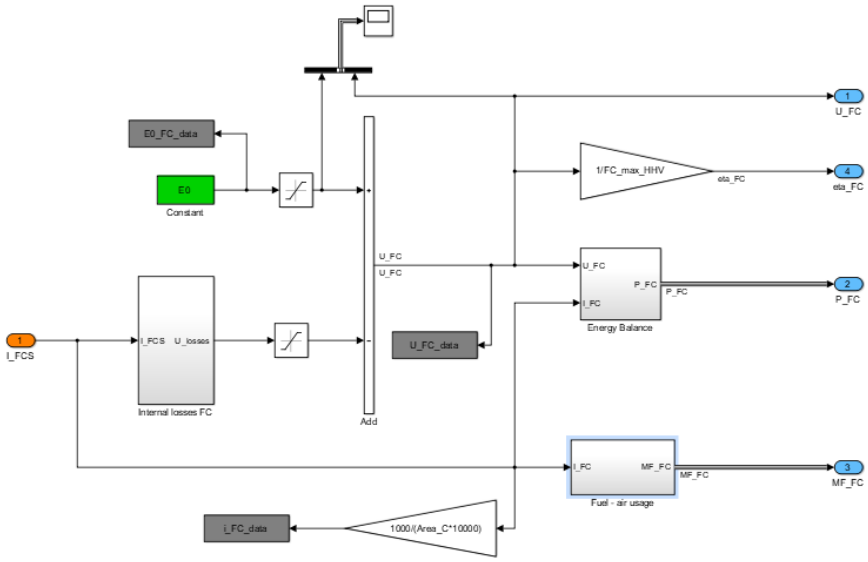
(A) "FC Stack" block

Inside the "FC Stack" block (see **FC Stack**), the characteristics of a single fuel cell are calculated first. Thereafter, by multiplying the number of fuel cells in the stack, the characteristics of the whole stack are acquired.



FC Stack

The calculation in “Single FC” (whose system layout is shown in **Single FC**. is based on Nernst equation **(2.2)**. The internal losses, including activation losses, Ohmic losses, and concentration losses are taken into consideration in “Internal losses FC” block.

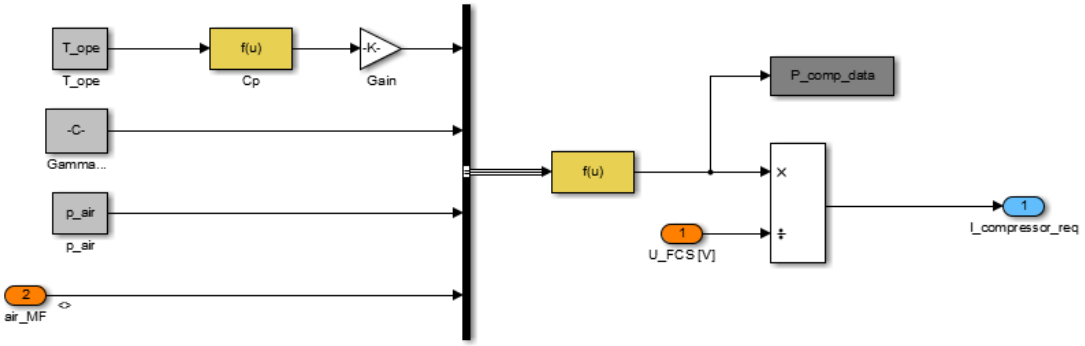


Single FC

The output efficiency (eta_FC) is calculated based on HHV of the fuel. Within the Energy Balance block, the power and efficiency of generating electricity, heat, and steam are calculated separately in the “Eta Overview” block. The “Fuel-air usage” block calculates the mass flow of both the fuel and the air.

(B) “Air compressor” block

Inside the “Air compressor” block, power demand is firstly calculated. By dividing it with the stack voltage, the current demand is acquired.



Air compressor