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Evaluation of system simulation tools by modelling a 100 kW PEM fuel cell system

Master's Thesis

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Abstract

The main purpose of this thesis is to explore and review the possibility of a 0D / 1D simulation to support the general fuel cell system design and development. The thesis also encapsulates the needs of the users by analyzing the type of use and adapting the system for it. The focus of this project is to model a fuel cell system. The scale of this project encloses to:

- Develop, build and verify models for the balance of Plant (Fuel (Anode) system, Air (Cathode) system, Coolant system). Implementation of a (simplified) controls strategy.
- Understand required component and measurement data for modelling and validation of the system.
- Evaluation of the potential to predict system behaviour and performance in real steady-state operation mode.
- Comparison of the evaluated approaches acc. to defined criteria and recommendations.

The model of the fuel cell system is designed and the system simulations are carried out in two distinct simulation environments. Modelon Impact and GT- Suite are the two simulation tools that are investigated. The simulation is first carried out in Modelon Impact simulation environment and the results are evaluated with how detailed and specific design can be generated. The same approach is carried out in GT- Suite. The above-mentioned software is compared on various parameters to improve the system simulation of fuel cells.

The thesis is intended to be a foundation for the design and simulation of a fuel cell and the working system around it. The results of this thesis are presented in a manner as to function as a foundation for the decision-makers. The results are based particularly on technical aspects, as the economic part is up to the decision-maker to look into.

Acknowledgement

I would firstly like to thank PowerCell Sweden AB for giving me this opportunity to carry out my Master thesis with them.

I would sincerely like to thank my supervisors at PowerCell, Volkmar Frick and Stefan Bohatsch for their constant guidance. The communication line was always open whenever I ran into a hiccup. They encouraged me to have a paper with my own work and steered me in the right direction as necessary.

I would also like to thank Prof Bengt-Erik Mellander of Chalmers University of technology. He has always welcomed any kind of doubts. I'm grateful for the wonderful feedback and valuable comments on thesis work. This has deeply benefitted the quality of my work.

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I would like to thank Marcus Åberg from Modelon and Christian Altenhofen from Gamma Technologies for their support with any issues or technical interruptions with the respective software.

Finally, profound gratitude must be expressed to my family and friends who were a strong pillar of support throughout the journey of my study and thesis. This accomplishment would not have been possible without them. Thank you.

Contents

List of Figures

List of tables

1. Introduction

1.1 What is a fuel cell?

A fuel cell is a device that uses the concept of electrochemistry to convert the chemical energy stored in hydrogen to electricity (Fig 1. 1). Traditional electricity-producing technologies involve multiple energy conversion steps:

- The fuel is first combusted where the chemical energy of the fuel is converted to heat energy.
- This heat energy is then used to convert water to steam.
- This steam then moves the turbine blades thus converting heat energy to mechanical energy.
- The turbine blades are connected to a generator that produces electricity and this process is the conversion of mechanical energy to electricity.

All these steps are skipped by the use of fuel cells as there is no requirement for the moving parts and multiple energy conversions which makes it far more efficient. This single trait has attracted a lot of attention towards fuel cells. Since it's a single step conversion, naturally it's assumed to be simpler and less expensive. But this is not yet the case as this technology is still new and is under development.[1]

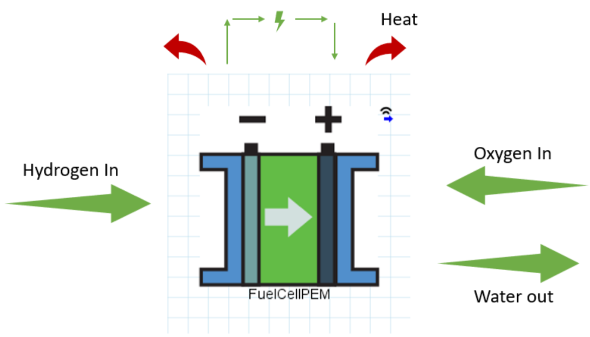

Fig 1. 1 Fuel cell

1.2 Basic principle

The first step towards the fuel cell was demonstrated with a simple experiment by William Grove in 1839.[2] Fuel cells' operation principle is quite simple. It follows the reaction as mentioned below.

$$2H_2 + O_2 \longrightarrow 2H_2O$$

One way to describe the operation of a fuel cell is that in a fuel cell, hydrogen gas is combusted as per equation 1.1 and the primary resultant of the reaction is electricity, water and heat. As it can be seen from Fig 1. 1, a fuel cell looks very much like a battery with an anode, cathode, membrane etc.. but it needs a supply of fuel and oxidant to produce electricity. The membrane is the key component of the fuel cell which has distinctive capabilities like being impermeable to gases and yet being conductive to ions while acting as an insulator to electrons. This membrane functions as an electrolyte and is compressed between the electrodes. There is a layer of catalyst at the interface of the electrode and membrane where vital reactions occur. The electrochemical reaction mentioned previously happens mainly on the surface of the catalyst. This can be seen in Fig 1. 2

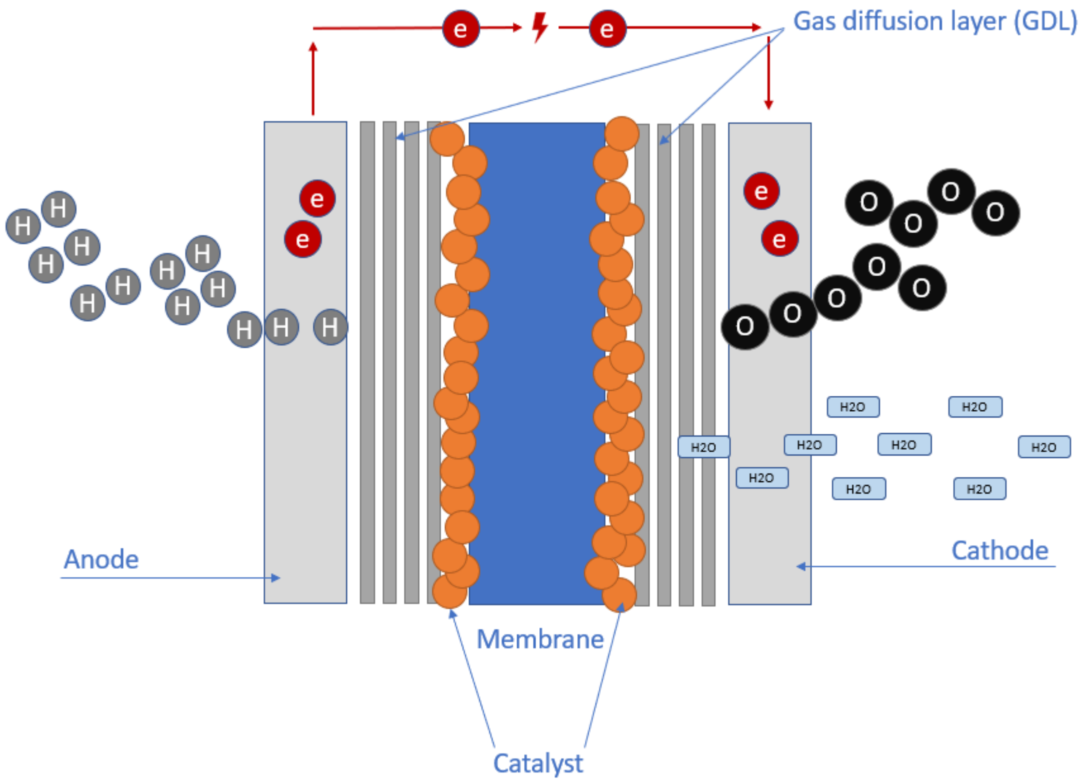

Fig 1. 2 Fuel cell working model with different components

Hydrogen gas is supplied to one side of the membrane where it splits into protons and electrons. The electrons travel through the electrically conducting electrodes and respective circuits producing electricity, while the protons pass through the membrane and react with oxygen and its electrons that are being supplied on the other end of the membrane thus producing water and heat. The water is pushed out on the side with an excess supply of oxygen.

The side on which hydrogen is being supplied is the negative side and is called an anode and likewise, the side with oxygen supply is positive and is called a cathode.

A single fuel cell produces less than 1V which is inadequate for numerous applications. The assembly of fuel cells is called a fuel cell stack. Several units of fuel cells are arranged in a fuel cell stack to match the voltage and power requirement as per different applications.[3]

1.3 Types of fuel cells

Different kinds of fuel cells are categorized according to the type of electrolyte being employed.

- Solid oxide Fuel cells(SOFC): They make use of non-porous, solid metal oxide electrolytes, often yttria-stabilized zirconia (YSZ).[4] They work in a temperature range of 800°C to 1000°C to make sure the ionic conductivity takes place by oxygen ions. This type of fuel cell is still in the development stage for large scale stationary power generation although quite a lot of development is seen for the small scale, portable type for the automotive sector.

- Phosphoric acid fuel cells (PAFC): They use concentrated phosphoric acid as an electrolyte. The concentration is nearly 100% and it's contained in a SiC matrix and is sandwiched between platinum catalysts on both sides of the electrolytes. Their operating range is between 150°C to 300°C. This type of fuel cell has been commercially installed in many places and is available for a 220kW demand of power.
- Molten Carbonate Fuel Cells (MCFC): This type of fuel cell employs a membrane in form of a matrix that contains electrolytes in which a combination of alkali carbonates are present (Li, Na, K). The matrix is made of $LiAlO_2$. The operation temperature of these fuel cells is in the ranges of 600°C-700°C as at these temperatures the alkali carbonate forms a highly ionically conductive molten salt. Due to this, the requirement of noble metals is avoided. They are still in the pre-commercial stage for stationary power generation.
- Polymer electrolyte membrane fuel cells (PEMFC): They use a thin proton conductive polymer membrane as an electrolyte in the fuel cells. They also use platinum as their catalyst with a working temperature range of 60°C to 80°C. They are the most developing type of fuel cell, with it being a potential candidate for mobile and stationary applications.
- Alkaline Fuel cells (AFC): As the name suggests this type of fuel cell use concentrated (85 wt%) KOH for high-temperature operation (250°C) and lower concentration (35 wt%) for lower temperature (120°C). This electrolyte is contained in an asbestos matrix for a membrane and uses noble metals, Ni, Ag etc as its electrocatalyst. This type of fuel cell has zero tolerance to CO_2 and is highly employed in space crafts.[1]

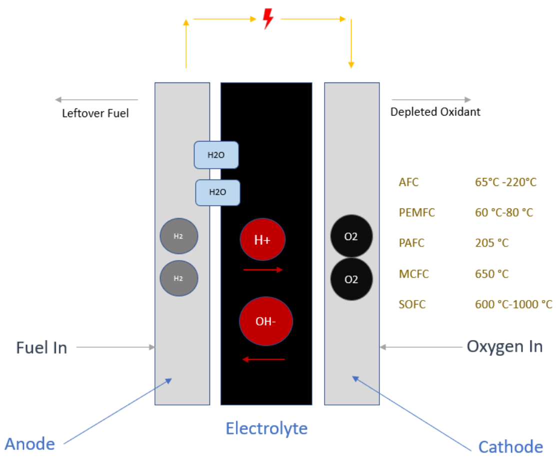

Fig 1. 3 Fuel cell types with their respective working temperature.

1.4 Need for Fuel cells and their Potential Uses

The various application of fuel cells along with their distinctive qualities make it a promising future technology. Fuel cell complements a conventional combustion engine but has positive attributes namely:

- The promise of high efficiency as there is no multiple energy conversion as discussed previously.
- Zero-emission as the only by-product for the reaction is water.
- Silent technology and a longer lifespan due to the absence of moving parts.
- Enhances energy security by avoiding dependence on conventional sources.
- Lightweight and small in size as compared to its competitor being batteries.

Fuel cells find their potential uses in Automobile sectors, Utility vehicles, Small scale power backup systems, Portable power, Space crafts, Locomotives, Airplanes and Small Ships and boats.[1]

1.5 Other parts of a PEM fuel cell system

Of all the types of fuel cells mentioned in the previous section, PEM has attracted a lot of attention in the recent past due to its prime applicability in automotive, small scale and portable energy-producing sectors. In this report, the focus will be primarily on the PEM type of fuel cell. A simplified PEM fuel cell system is depicted in Fig 1.4.

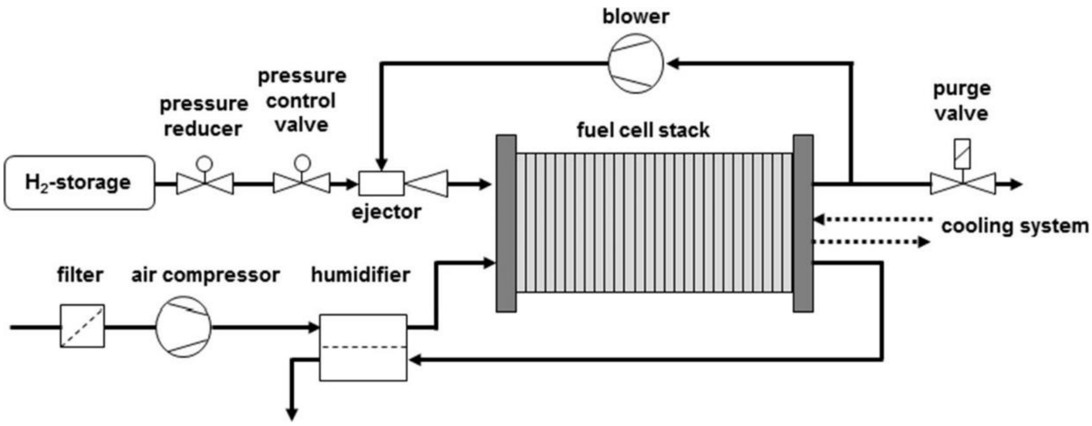

Fig 1. 4 Simplified PEM fuel cell system[5]

A fuel cell's key components are the electrodes, membrane (electrolyte) and catalyst as discussed previously. However, there are other extra parts and components to make up an entire fuel cell system. These components are referred to as the balance of plant components.[2] Some of the important components are compressors which are used to drive the flow of air and fuel through the stack. The recirculating blower is employed for the circulation of H_2 for better fuel utilization. Compressors are often accompanied by intercoolers to maintain the temperature of the inlet. Fuel storage is also a component required for a system using hydrogen. For the coolant system, pumps are used to circulate the coolant and tanks as the buffer storage. A humidifier is one of the key components of the system which maintains the humidity of the stack. Various control valves, pressure regulators and controllers are also part of the extra components. These components help in connecting the sub-systems to maintain the proper function of the fuel cell stack.[2] Some of the components explained here haven't been depicted in the figure, but have been modelled and explained in the later sections.

2. Modelling overview

In the new era of engineering which is bestowed upon us, research and testing are happening together at the same time. The future of the engineering of physical systems is especially complex and demands advanced modelling capabilities. The gaps in physical modelling and high barriers to entry have prevented many organizations from deploying and engaging in the benefits of simulation.[6]

In a PEM FC hydrogen and oxygen reacts electrochemically to produce water, electricity and heat. Many interconnected complex processes occur during the operation of PEM FC. Processes like Mass, Heat, Electrochemical and Ionic transport occur simultaneously. To truly understand the working of fuel cells, one must utilise the fundamentals of modelling which is in turn based on physics models from the data of observed experiments.[7]

Over the last few years, the publication frequency on the topic of fuel cell system modelling has increased. In this review, the main focus is on 0-D and 1-D models. 0-D models are defined by the geometric dimensionality and simple equations making the model empirical.[7] The 1-D model accounts for complex effects encapsulating effects taking from simple equations to complex expressions obtained from physical characteristics. The amalgamation of other non-geometric effects like macroscopic and microscopic (amount of H_2 being consumed, Stoichiometry etc) along with the frequency, complexity, detailing and designing scope has also increased. The added advancement of technology and fast computing has only boosted the entire concept of modelling and simulation by reducing the limitation and constraints. Currently, some models have the detailing of the fuel cells in 2-D and 3-D accounting for the effects of flow in the direction of the flow and across the direction of flow along with effects accounted in 1-D and 0-D.[7]

The main aim of this review is to evaluate two different simulation software for the modelling of fuel cell systems by modelling the same fuel cell system in both environments. Direct comparisons are generally hard to make as they might differ in the approach and detailing of the model. One of the models might be good in a certain region (ex: electrode, catalyst and its kinetics) whereas the other might be good at other regions (ex: membrane, humidity, conductivity response to the current density). They cannot be 100% accurate and this is not the target of evaluation. But the key is to bridge the gap between the real physical system and the system model and thus judging the accuracy of the tool.

3. Objective and Problem Description

The purpose of this thesis is to evaluate the software tools namely GT-suite and Modelon Impact which is carried out in a structured manner that is described below:

- Literature Survey: The initial few days were spent on a literature survey where some of the basic system designs of the fuel cells were explored and the basic idea was grasped. The process and instrumentation diagram of a particular system (MS-100) was provided by PowerCell. This design was to be modelled on the respective software.
- Explore the simulation software and understand its functionality and detailed available libraries. This involves understanding and diving deep into the way of the implementation of auxiliary components and their behaviour. These components are then used to build up the entire system.
- Analysis and validation of the designed system model(including the subcomponents): Characterizing the model based on its practicality, level of detailing and application of the details i.e mapping, equations involved, slopes and ease of use, that is basic modelling.
- Evaluation of the simulation tools, based on the gaps they fill with different approaches in different tools. Assessment benchmarks will be based on:
    - Functionality.
    - Workflow and ease of use with components.
    - Documentation on how the components are implemented.
    - Level of detailing.
    - Ascending the approaches of modelling.
    - How direct or indirect the approaches are for the design.
    - Technical support for the software developers.
- Thesis report and documentation.

4. Introduction on the Software Tools

In this section, a brief introduction about the software tools along with their background, origin and uses is given.

4.1 Modelon Impact

4.1.1 What is Modelon Impact and its Background?

Modelon Impact is a simulation software that is a product of the company Modelon. Modelon presents systems modelling and simulation software that speeds up innovative products, advancements, and activities in a range of industries. Modelon Impact is a 0D/1D dynamic system simulation software featuring several proven models and components spanning across a broad spectrum of applications. It is a cloud-based interface that features the utilisation of a collaborative web browser. This company is headquartered in Lund, Sweden with a global reach. Modelon claims that its an expert industry leader in model-based systems engineering with a focus on leveraging open standard technologies. The open standard technology being discussed is Modelica.[8] This open standard enables the users to exchange models with any Modelica-compatible tool and allows the utilization of the models for simulation and analysis without the need for a specific tool.[8] For the purpose of this thesis, Modelon Impact version 1.1.1 is used.

4.1.2 Stages involved to obtain convergence

There are mainly 3 stages involved in arriving at a solution, see Fig 4. 1

- Component Library: A person with experience in system simulation would be familiar with the component library which supplies a wide range of components with different functionalities. These are used in a combination of different kinds to form a system as per requirement.[9]
- Workspace of Modelon Impact: This is a space where the model is designed. In Impact, there are 2 ways to have this design implemented, i.e. either via coding (which would require knowledge on coding) or via drag and drop method (drag components from libraries and drop them in the canvas and connect the inputs and outputs of the components on the Graphical User Interface(GUI)). This makes the software interestingly flexible of having a mix of capabilities of both code layer and GUI. Although the trend in the simulation tools is moving towards drag and drop methods, it is interesting to have an option to also use the code layer. It allows the user to have the flexibility to build their own model based on the existing library but with additional functionality which can be re-used in the future.[9]
- Development of application and engine: In this way, you build an engine that enables the compilation of your designed model to make it run. For ex: A user's requirement may be to just have him plug in some input values and get an output value without spending time on the technical details.

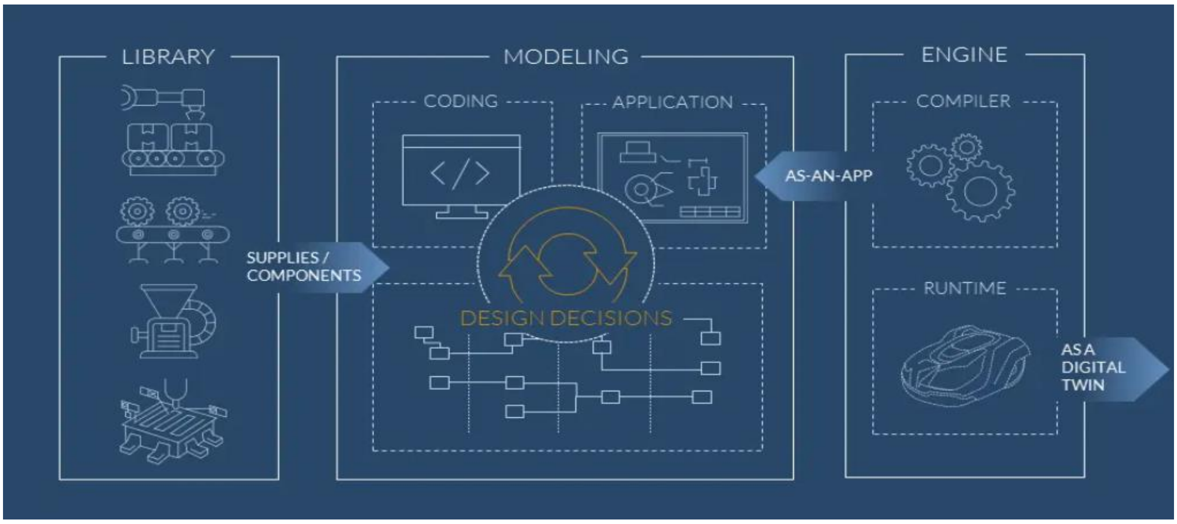

Fig 4. 1 Diagram representation of the 3 stages[9]

4.1.3 Uniqueness of Modelon

In the current scenario, among a lot of system simulation tools, there is a huge gap in technical expertise. It ranges from the fact that it's either purely a drag and drop interface or high expertise of technical knowledge and coding. With Modelon Impact, there is a platform that enables the mix and match of both thus bridging the gap for engineers in system simulations. The engineer working with the system simulation is able to decide about the implementation of the model based on the behaviour of the component. Behaviour is actually quite an important factor when there is an existence of different domains and disciplines, and having them integrate into a system as a whole.[9]

4.2 GT-Suite.

4.2.1 What is GT-suite and its background.

GT-suite is a popular system simulation tool that is used in many industries worldwide. It is a multi-purpose environment consisting of many physical libraries with both complex and fundamental components that can be used to build system models with an infinite variety and thus making the lives of engineers easy and empowering.[10] The application of GT- suite spans over a wide range of industrial variety for ex: Thermal management, Multibody mechanics, Fluid systems, Propulsion systems to name a few. GT-suite is a 0D-1D simulation tool with solutions for real-time simulations and control systems simulations. GT-Suite is a licensed product of Gamma Technologies. Gamma Technologies is headquartered in Westmont Illinois, USA. The modelling of the fuel cell is carried out in version 2021 of GT-Suite.

4.2.2 Uniqness of GT-Suite

GT-Suite is a unique tool based on the fact that it's an all in one CAE tool. It is a leader in the 0D-1D level of modelling, but it also has the ability to work as a detailed 3D modelling tool with a built-in FEA and CFD. Finite element analysis (FEA) is a process of performing simulations and assessing the behaviour of a part of an assembly or an entire assembly for given conditions. Engineers utilise this tool to perform simulations of physical phenomena and as a consequence of which there is a reduction in the development of physical prototypes. FEA also allows optimization of components of assembly as a part of the design of the project.[11] Computational fluid dynamics (CFD) is a procedure of modelling physical phenomena mathematically and numerically solving them with the assistance of computer prowess.[12] GT-Suite can be complemented with a CAD design as well. GT becomes more powerful by integrating 3D components with high fidelity into a 0D-1D level model with the feature of supplying all the accurate data from boundary conditions and transient conditions between the subsystems. In addition, GT has built-in features such as an optimizer and design of experiments functionality which makes it convenient and attractive for engineers.[13]

5. Detailed workflow and modelling

This section contains, discussion regarding the exact workflow and how each component is modelled and what equations the modelled components depend on, starting with the workflow that was followed during the duration of this thesis.

5.1 Workflow

Explore both the Simulation environment and its respective libraries

↓

Learn the component modelling and mapping

↓

Establish boundary conditions across the components and validate them with the supplier data

↓

Repeat the same for all the components in the system

↓

Model the system design of a 100kW system using the elements and components of the libraries

↓

Fine-tune the components with measurement data and accurate geometry

5.2 Auxiliary components

A fuel cell stack cannot function as a stand-alone component and needs a system around it that is integrated together. A fuel cell system has various combinations of auxiliary components like pumps, heat exchangers, compressors, humidifiers, electrical components and control systems in place to engage in the right amount of dispensing of air and hydrogen and coolant as explained in section 1.5.[3] Some of the components being used in the designed system are listed below.

5.2.1 Compressors:
Compressors are mechanical devices that increase the pressure of the fluid by reducing the volume of the fluid and thus increasing the density. The compressors allow and account for the transport of the fluid through a series of pipes and any other components.

The compressor is modelled with the knowledge of 4 important parameters that are given as input by the user/developer. The 4 important parameters that are defined by the developer with the help of data from the component supplier are mass flow rate, pressure ratio, compressor speed and efficiency for the different conditions. Based on these parameters the component models a dynamic state mass and energy balance. This step is called the characterization of the compressor. A function called character map is provided wherein the performance of the compressor is characterized according to the input parameters. A character map is basically a lookup table. The input parameters are nothing but the manufacturer data that needs to be corrected before it can be entered. The corrected parameters are based on the following equations:

$$RPM_{corrected} = RPM_{actual} / \sqrt{\frac{T_{inlet-total}}{298}}$$

$$\dot{m}_{corrected} = \dot{m}_{actual} * \sqrt{\frac{T_{inlet-total}}{298}} / \frac{P_{inlet-total}}{100}$$

Where RPM (rotation per minute) is the speed of the compressor, T is the temperature, $\dot{m}$ is the mass flow rate of the fluid and P is the pressure.

Modelon Impact

In Modelon Impact there are different types of compressors namely, positive displacement compressor, dynamic compressor and signal defined compressor. In this case, a dynamic compressor is chosen amongst the 3 types, see Fig 5. 1. The dynamic model of the compressor is modelled with two 2D lookup tables namely the Isentropic efficiency table and Mass flow table, see Fig 5. 2 and Fig 5. 3. The values from these lookup tables are directly used without any other further processing.

The extrapolation outside the map region is based on the last 2 points on the map. The map is an algebraic model i.e it does not bring any dynamics to the model. The isentropic efficiency is used to calculate the torque which is then used to calculate power. In the mass flow table, the mass flow of the fluid is characterized by different pressure ratios and compressor speed.

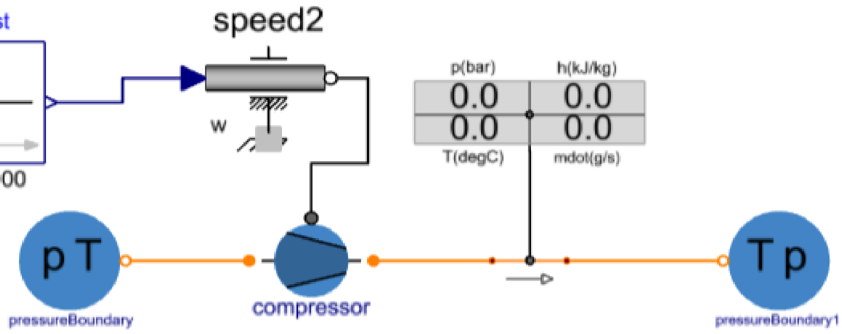

Fig 5. 1 Compressor model in Modelon Impact

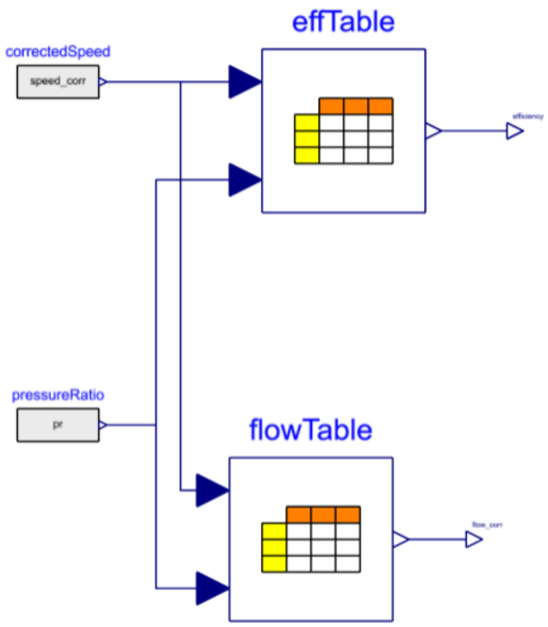

Fig 5. 2 Character maps for the compressor.

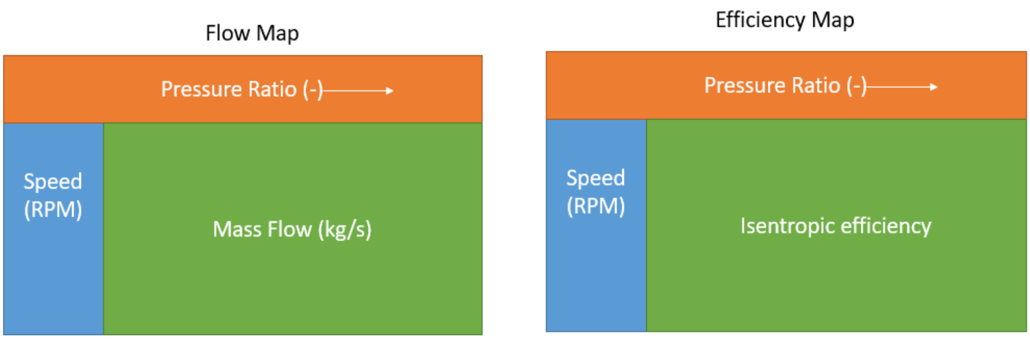

Fig 5. 3 Example of character map for a compressor

The compressor is validated with the supplier data. The supplier data was given in the form of data points which are plotted in Excel. This raw data is then pre-processed in a readable manner before feeding it to Modelon Impact. The modelled graph in Impact is converted to a CSV file and is imported to excel for comparison and to see the accuracy.

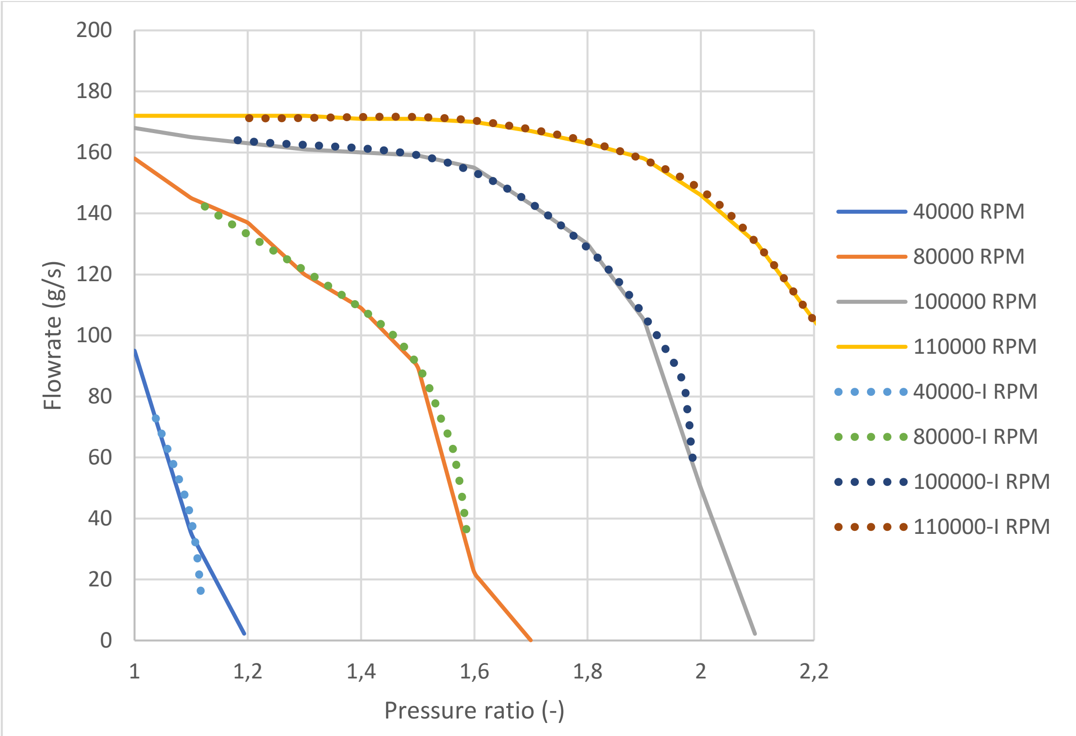

Fig 5. 4 Comparison of Supplier data with modelled data-(Flow table)

In **Error! Reference source not found.**, the solid line is Modelon Impact modelled data, and the dotted line represents the raw unprocessed data. The accuracy can be concluded as high.

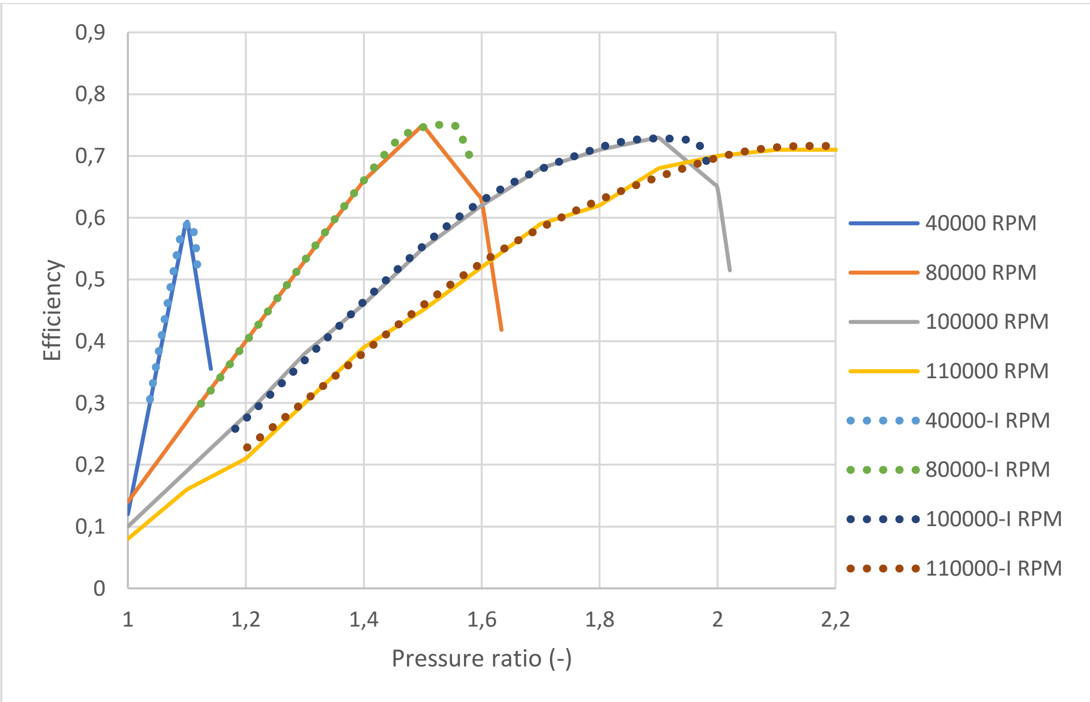

Fig 5. 5 Comparision of Supplier data and modelled data-(efficiency table)

Similarly, in Fig 5. 5 for efficiency characteristics, the dotted line represents the raw data and the solid line is modelled data from Modelon Impact. Similar to the previous fig, it can be seen that efficiency has been mapped with good precision. But the extended solid line represents an extrapolation by the software. This may lead to unreasonable results if operated in those ranges.

GT-Suite

In GT-Suite, Unlike the procedure in Modelon impact, there is only one compressor model, see Fig 5. 6. The type of compressor can be selected within the compressor component. After which the reference pressure and temperature are defined along with wheel diameter, Gas-constant and specific heat, see Table 5. 1. Once this preliminary data has been defined, then data for speed, mass flow, pressure ratio and efficiency need to be defined, see Fig 5. 7.

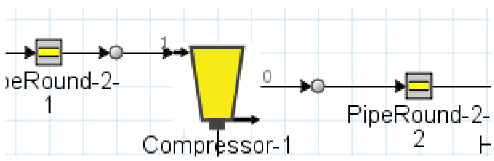

Fig 5. 6 Compressor model in GT-Suite

Attribute	Unit	Object Value
Compressor Type		radial
External SAE File Name		ign
Create Pre-Process Plots?		☑
Pre-processing Message Level		simple
Reference Pressure	bar	1
Reference Temperature	C	25
Reference Gas Constant	J/kg-K	287
Reference Ratio of Specific Heats		def (=1.4)
Wheel Diameter	mm	34.7

Table 5. 1 Preliminary data input

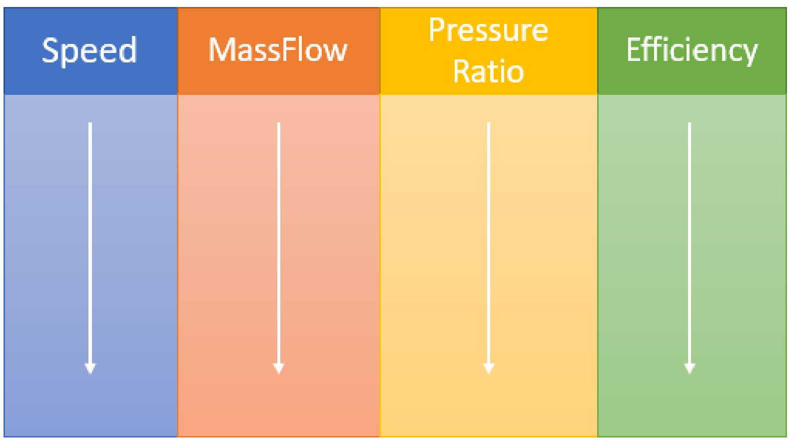

Fig 5. 7 Character Map example

One positive point in favour of GT mapping is that one can have the data in any unit and it can be copied from excel directly to the map table and then the units can be converted. GT-suite comes with a pre-processing tool that generates the graph based on the input data. The data need to be pre-processed before feeding it into GT-Suite as well. And again comparing it with the manufacturer data we have a graph as shown below.

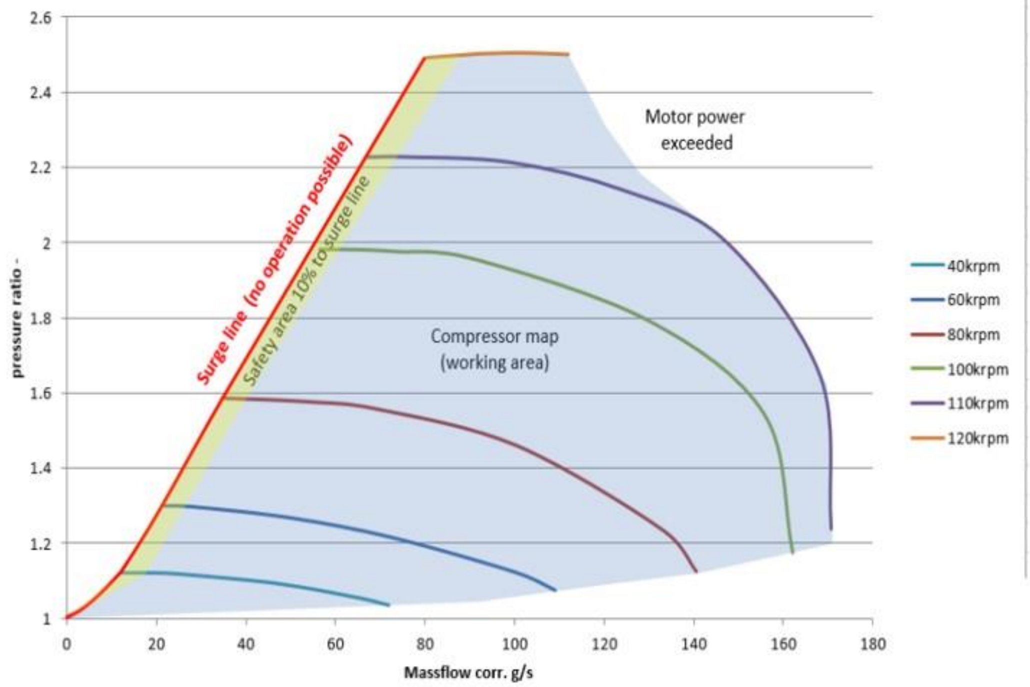

Fig 5. 8 Manufacturer Data

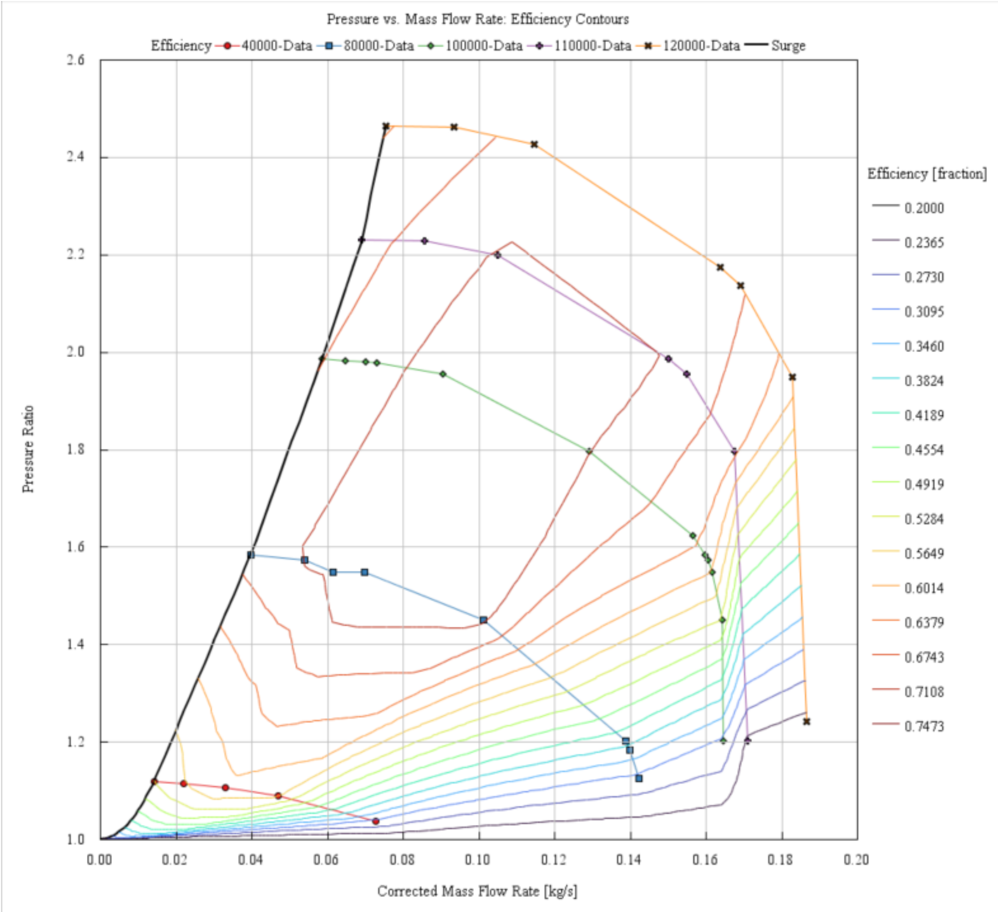

Fig 5. 9 Character Map generated by GT-Suite

From Fig 5. 8 and Fig 5. 9 we can see quite a good precision in the mapping as the data is extracted from Fig 5. 8 and fed into the software, where mass flow corrected is given by the equation

$$\dot{m}_{\text{corr}} = \frac{\dot{m} \cdot \sqrt{\frac{T}{298\text{K}}}}{p/1\text{bar}}$$

5.2.2 Pumps: Pumps are mechanical devices that push the fluid from a region of low pressure to high pressure. Essentially, the pump imparts mechanical energy to the fluid by the means of the centrifugal force of its impellor. Pumps are used to force the fluid further into the pipeline of the system.[14] Sometimes, pumps and compressors are used interchangeably. One way to understand it better is that a **pump** moves fluid (liquid or gas) from one place to another. The **compressor,** on the other hand, squeezes the gas to a higher density whilst moving it to another place.[15]

Modelon Impact

In Modelon Impact, the modelled pump describes a centrifugal pump with a rotational mechanical connector as a shaft, see Fig 5. 10. The model uses a characteristic map that defines the pressure rise and volumetric flow rate. Volumetric flow rates and pressure rise is provided with sufficient data points to cover a range of operation. Based on these values the functionality of the pump is defined. The curve is linearly interpolated between the points and extrapolated based on the last two specified points for higher flow rates. The calculation of the efficiency of the pump can be characterized by efficiency characteristics, power characteristics or torque characteristics depending on the kind of data that the user has. In this case, we will discuss characterizing by Power characteristics. Power can be characterized by a table function that correlates pump power consumption and volumetric flow rate. Note: These data sets are entered for different speeds of the range the pump is supposed to work. For pump speeds outside the range of table data, affinity laws are used based on the nearest rotation speed from the data set(depicted in Fig 5. 12). The affinity law is defined by the following equation:

- Flow vs Speed: $\frac{Q1}{Q2} = \frac{N1}{N2}$
- Head vs Speed: $\frac{H1}{H2} = \left(\frac{\mathrm{N1}}{\mathrm{N2}}\right)$ ^2

where Q corresponds to the flow rate of the pump, N is the speed of the pump and H is the head of the pump.

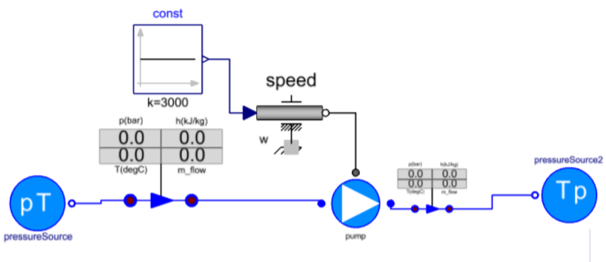

Fig 5. 10 Model of a pump

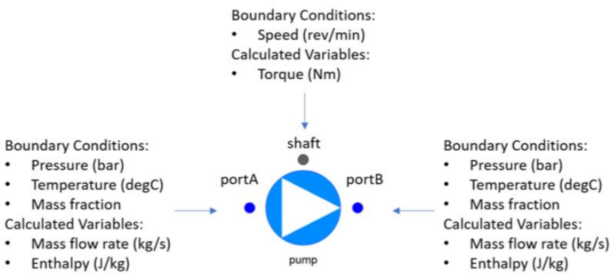

Fig 5. 11 Boundary conditions of the pump

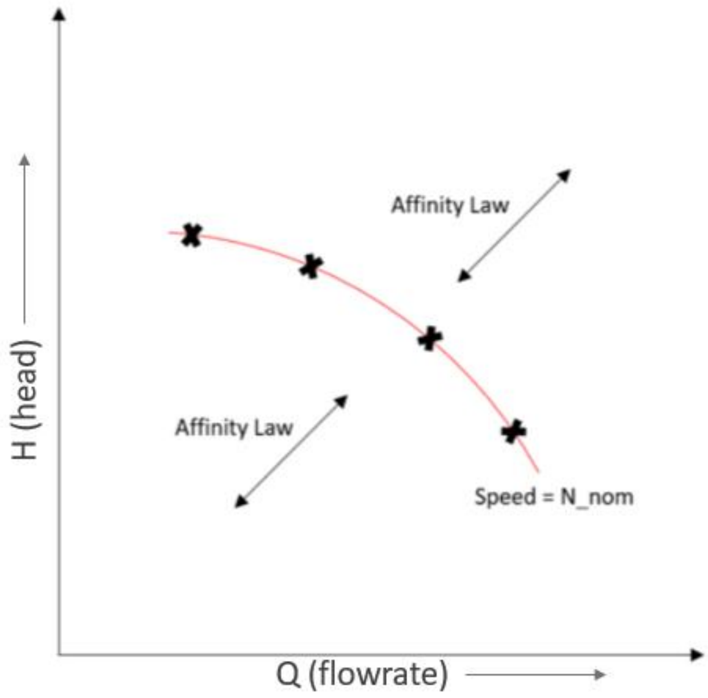

Fig 5. 12 Affinity law

Fig 5. 12 illustrates affinity law graphically, where the x-axis depicts the flowrate Q and the y-axis depicts the head of the pump H as explained in the equation earlier.

Once the pump is modelled, it was validated with the manufacturer data. And this is compared diagrammatically in the figure.

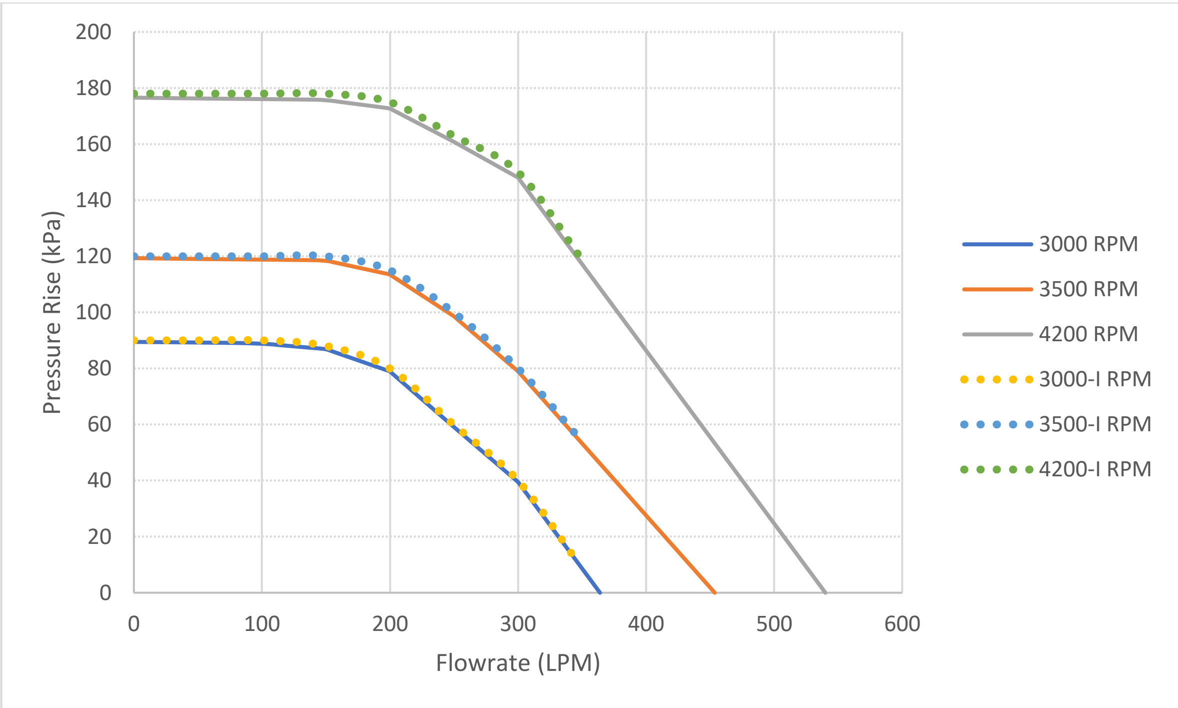

Fig 5. 13 Modelon Impact modelled data compared to supplier data

Here in Fig 5. 13, the solid line represents, data modelled by Modelon Impact and the dotted line is the supplier data that is fed in. It can be concluded that the validation is accurate. The solid lines extend beyond the dotted lines, this is because Modelon Impact uses an inbuilt extrapolation.

GT-Suite

In GT-Suite the mapping of the pump is a much simpler process. The template is modelled based on performance measured data that correlates pump speed, flowrate, pressure rise and efficiency all together in one table. It is used to model a mechanical pump with different imposed speeds. And similar to compressors mapping, the units are quite easily convertible making it easier to input the data. See Fig 5. 14

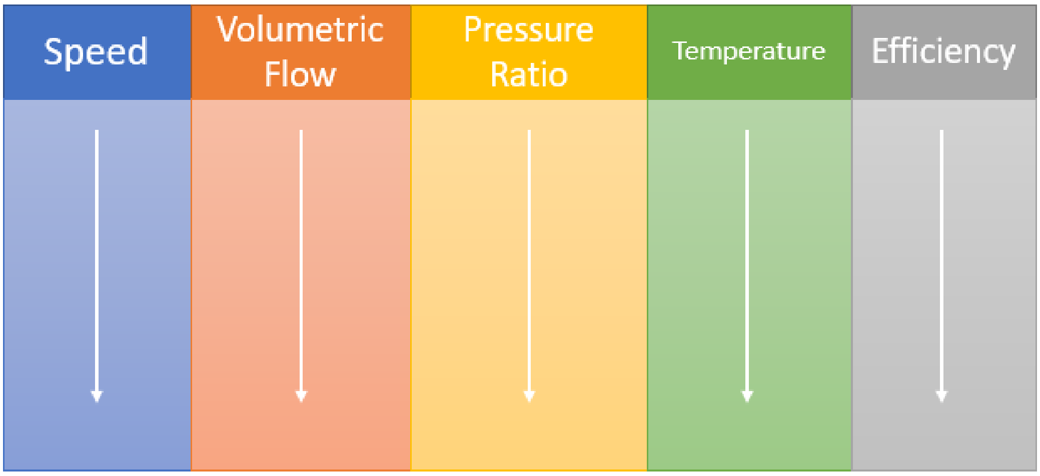

Fig 5. 14 Pump Character mapping example

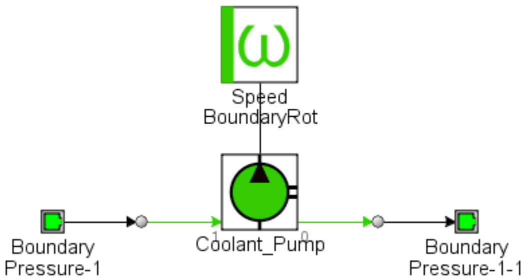

Fig 5. 15 Pump Model

Once this data is input, the pump is pre-processed and compared to the manufacturer data.

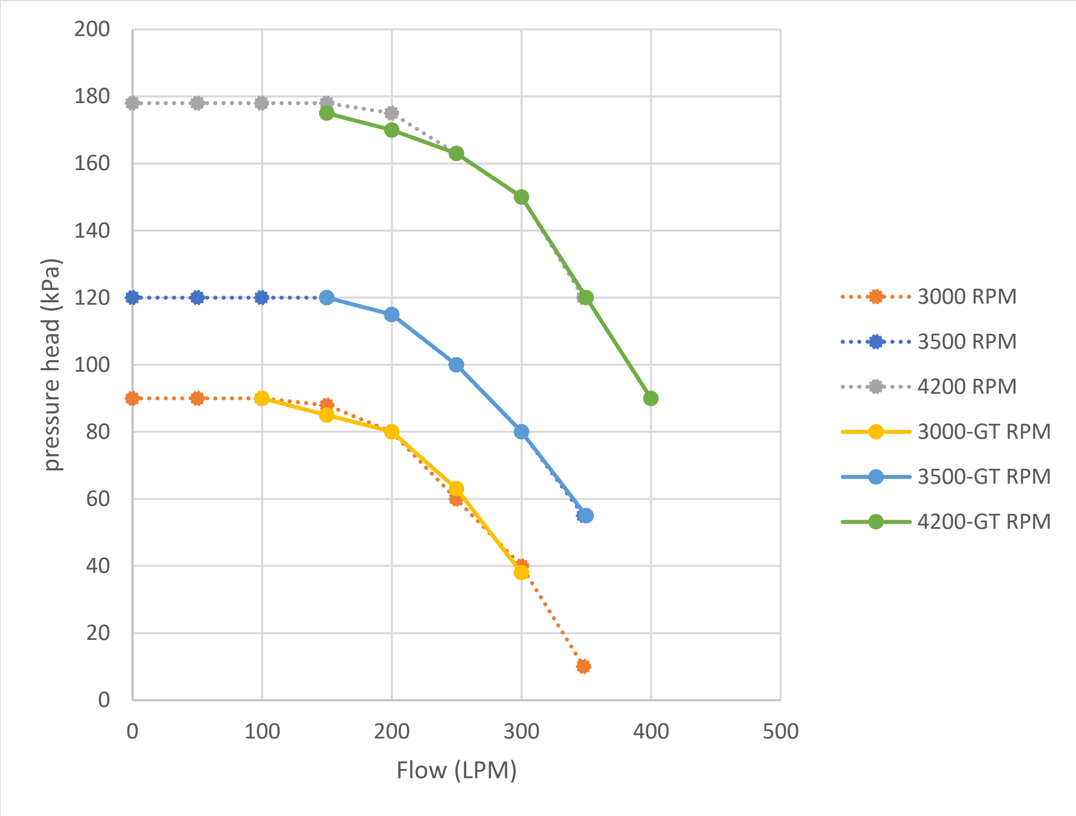

Fig 5. 16 Compared data from the manufacturer and pre-processed GT-Suite data

From Fig 5. 16 it can see that the accuracy is quite good with the comparison. The solid line represents GT-Modelled data and the dotted line is the supplier data.

5.2.3 Heat exchanger: A heat exchanger is a system that enables the exchange of heat between 2 fluids. Heat exchangers can be used in both cooling and heating processes.[16] The fluid is usually separated by a wall to transfer heat without the fluid mixing. The exchanger used in this case is a counter-current flow heat exchanger which is defined by the parameterization of the geometry of the primary side and the secondary side of the heat exchanger. The efficiency or effectiveness of the heat exchanger is a function of the surface area of the wall and the temperature difference between the two fluids with heat transfer coefficient.[17]

Modelon Impact

In Modelon Impact the heat exchanger is modelled using a Number of Transfer Units (NTU) approach.[18] NTU method is used to calculate the heat transfer in the heat exchangers when there is insufficient information. The NTU method holds good when the information on the inlet and outlet temperatures aren't known. If the temperatures are known, the Log-mean temperature difference (LMTD) can be calculated.[19] The heat transfer characteristic is defined by the total heat transfer coefficient which is a function of the geometries of primary and secondary flow channels and the area of heat transfer wall from which NTU is decided. With the known value of NTU, the effectiveness of the heat exchanger is determined, see Table 5. 2 Primary and secondary side geometries. The actual heat transfer is thus calculated based on the effectiveness. The mass flow is defined by a friction model of the heat exchangers.

Primary side geometry		
n_channels_prim	25	
L_prim	0.3	m
Dhyd_prim	0.05	m
A_prim	0.00196	m^2
V_prim	n_channels_prim * L_	m^3
A_heat_prim	1	m^2
Secondary side geometry		
n_channels_sec	25	
L_sec	0.3	m
Dhyd_sec	0.04	m
A_sec	0.00125	m^2
V_sec	n_channels_sec * L_s	m^3
A_heat_sec	1	m^2

Table 5. 2 Primary and secondary side geometries

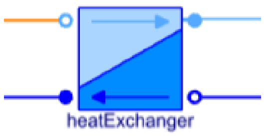

Fig 5. 17 Heat exchanger model

In this project, a heat exchanger is used as an intercooler after a compressor to cool the fluid down and once again in the cooling circuit to cool down and maintain the temperature of the fuel cell stack. It is used as a heat sink for both high temperature and low temperature cooling. In the system, with the knowledge of the temperature of the fluid downstream of heat exchangers, the geometry is calibrated to achieve this temperature.

GT-Suite

In GT-suite, the heat exchanger is quite easy to use model. The key parameter to be defined is the temperature of the coolant and it is also required to enter the outlet temperature of the fluid to be cooled. Then another parameter that is to be defined is the diameter which can also be set as 'def' which automatically takes in the value of the diameter of the component upstream of it or use a specific diameter for the heat exchanger thus imparting a pressure drop over the component accordingly. Based on the above-mentioned parameters, the cooling or heating duty is calculated. It also has a parameter to input the heat exchanger outlet temperature ratio of the heat exchanger, which allows it to calculate the design parameters to build an actual heat exchanger, see Fig 5. 18 and Table 5. 3.

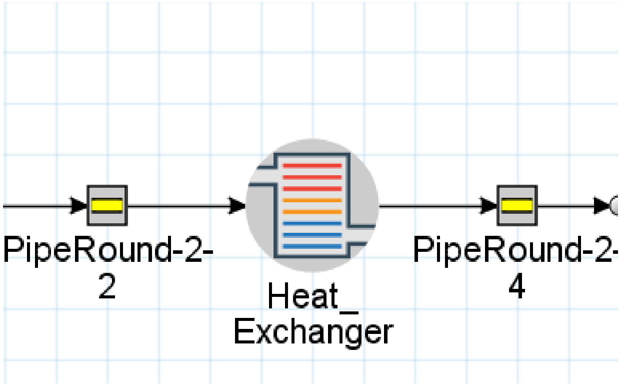

Fig 5. 18 HeatExchanger model

Attribute	Unit	Object Value
Diameter	mm	60
Forward Discharge Coefficient		def
Reverse Discharge Coefficient		def
Imposed Fluid Temperature	C	70
Heat Exchanger Outlet Temperature Ratio		ign
Coolant Temperature	See Case...	[T_Coolant_init]
Imposed Temperature Location		Downstream

Table 5. 3 Input parameters of Heat Exchanger

5.2.4 Humidifier

5.2.4 Humidifier: Humidifier is a device that essentially exchanges moisture between the dry and the wet gas streams. It also exchanges heat between the fluids in the humidifier. PEM fuel cells have membranes that need hydration to maintain high ionic conductivity and durability. It is actually useful to have the humidity of the cell membrane to unity where the ionic conductivity is optimum. Since the electrochemical conversion in a fuel cell results in the generation of water, membrane humidifiers are the right choice of humidifiers which offers the benefit of utilizing the water-saturated air at the exhaust of the cathode side. During the operation of the fuel cell stack, the temperature rises to nearly 80°C. Thus, the humidifier acts as a balance ensuring the humidity and the temperature are in check upstream of the fuel cell stack.[20]

Modelon Impact

In Modelon Impact, the humidifier is modelled as a gas-gas humidifier that is defined exactly like the heat exchanger mentioned in the previous section. The humidification is calculated on the secondary side using dummy dynamics for water diffusion (lumped humidifier). The water transfer/humidification process is driven by the saturation conditions along with the conditions of the air at the secondary inlet. For better understanding, the primary side is modelled as dry air and the secondary side is modelled with water-saturated air, see Fig 5. 19

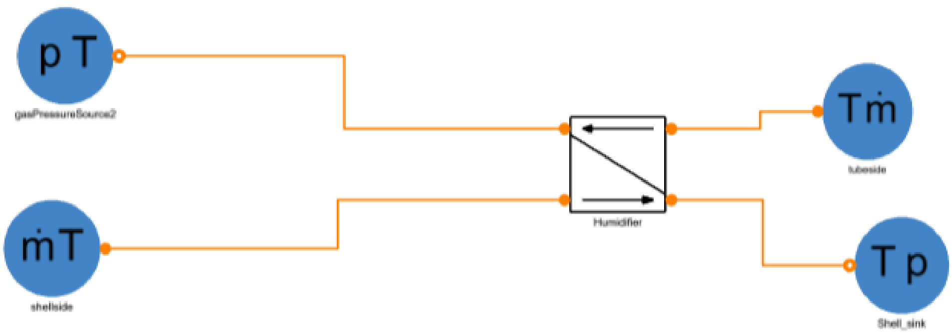

Fig 5. 19 Humidifier Model

This is then validated against manufacturer data to see how accurate the model can be. Since the humidifier model was a bit complex to model, the data points were simulated individually and plotted in excel, see Fig 5. 20. The airflow has a unit of sLPM which stands for standard litres per minute.

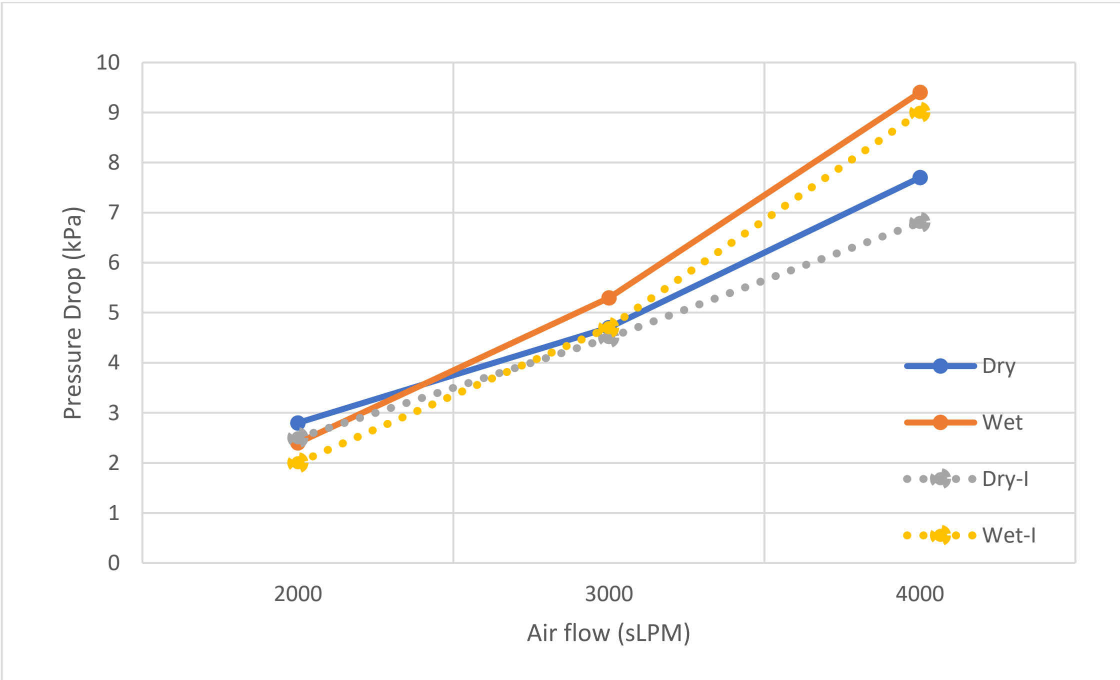

Fig 5. 20 Data validation - Pressure drop. The solid lines are the modelled data and the dotted line represents the supplier data.

From Fig 5. 20, the conclusion can be drawn that the model matches the supplier data with fair accuracy. The largest deviation is about 1kPa at 4000sLPM which is small compared to the total operating pressure of 7.7kPa at that point.

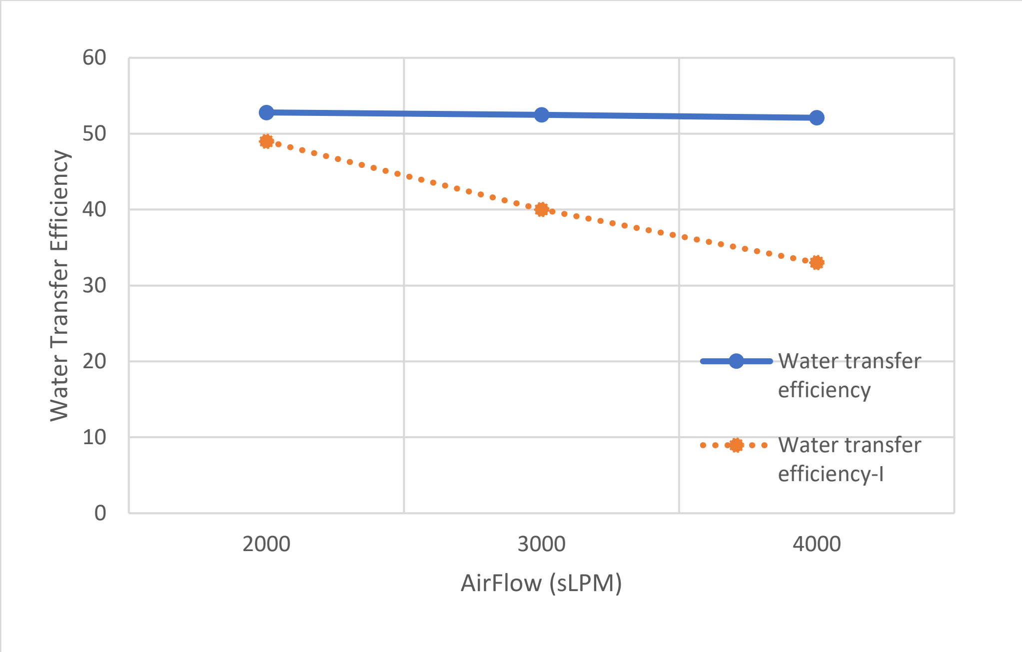

Fig 5. 21 Data Validation - Water transfer efficiency. The solid line represents modelled data and the dotted line represents the supplier data.

From Fig 5. 21 water transfer efficiency in the model is higher than the supplier data. This may arise due to the fact that the model assumes the vapour saturation on the dry outlet. The solid line represents modelled data and the dotted line represents the supplier data.

The humidifier model used in this project is a beta model which is lumped i.e not a discretised model. During the testing of the humidifier, issues/bugs in the calculation of outlet temperatures were found which was reported to the software development team. Unfortunately, the fix for this is anticipated beyond the time frame of the thesis. Hence a heat exchanger is used in the system model in place of a humidifier. The same validation of the pressure drop is carried out and is implemented. The bug fixes and a discretised humidifier model is in the development stages and will be released in the upcoming updates.

GT-Suite

In GT-suite the component used to model a gas-gas humidifier is of shell and tube type. This component is primarily intended for fuel cell modelling. In this component, the water transfers from the wet side to the dry side which is driven by the humidity difference across the membrane which in our case is Nafion. A basic heat transfer is applied to correlate the wet and the dry sides, see Fig 5. 22

An isolated humidifier model is set up and tested with specific boundary conditions. It is defined by its geometry as shown in Table 5. 4. It is made of discrete elements (subassembly) as shown in Fig 5. 23.

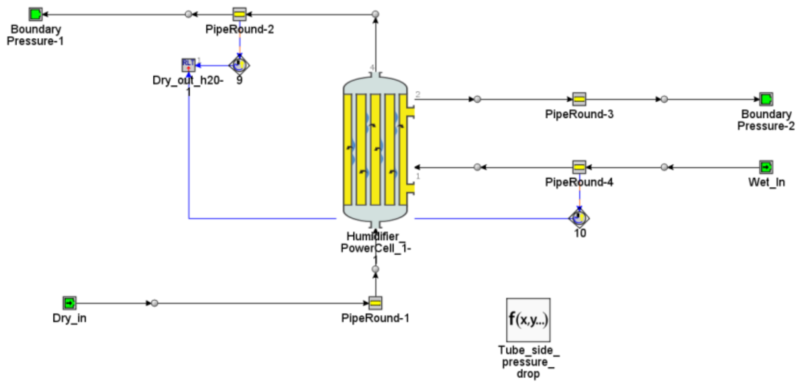

Fig 5. 22 Humidifier Model

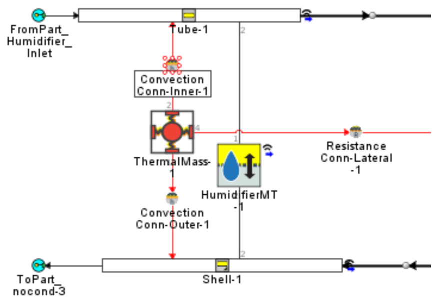

Fig 5. 23 Humidifier subassembly

From Fig 5. 23 we see two pipe objects which describe the tube side and the shell side of the humidifier. The two icons connecting the pipe objects depicts heat transfer and humidity transfer using a Nafion membrane.

Attribute	Unit	Object Value
Geometry		
Inner Diameter of Shell	See Case...	[shell_dia]
Inner Diameter of Tube	mm	0.8
Tube Membrane Thickness	mm	0.1
Number of Tubes		4320
Number of Shells		18
Length	mm	290

Table 5. 4 Geometry of the humidifier

Once the humidifier is geometrically calibrated with the appropriate boundary conditions, it is validated with the supplier data as done for all the other components.

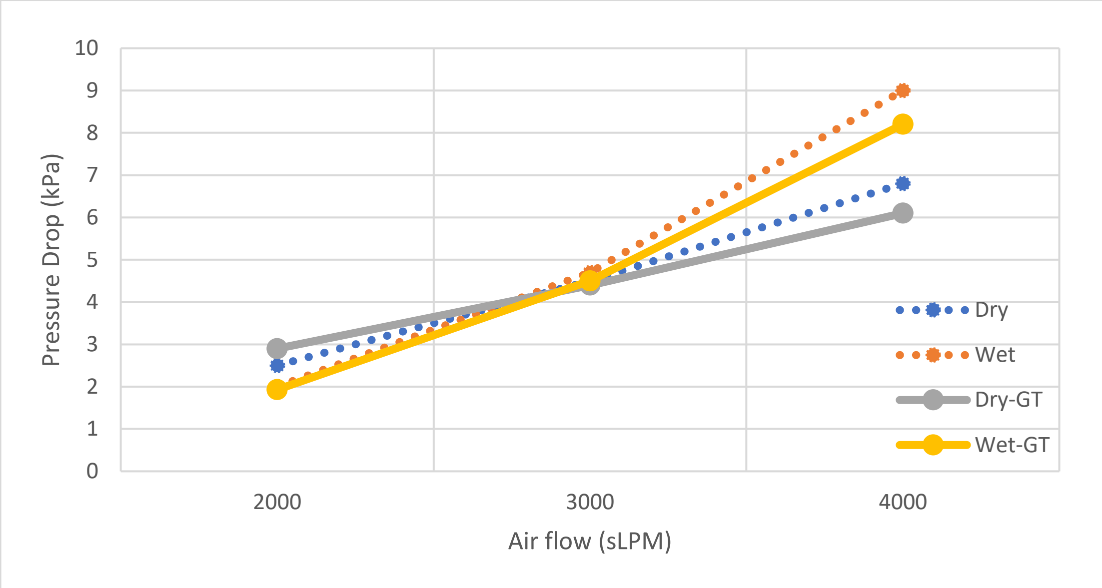

Fig 5. 24 Data Validation – Pressure drop

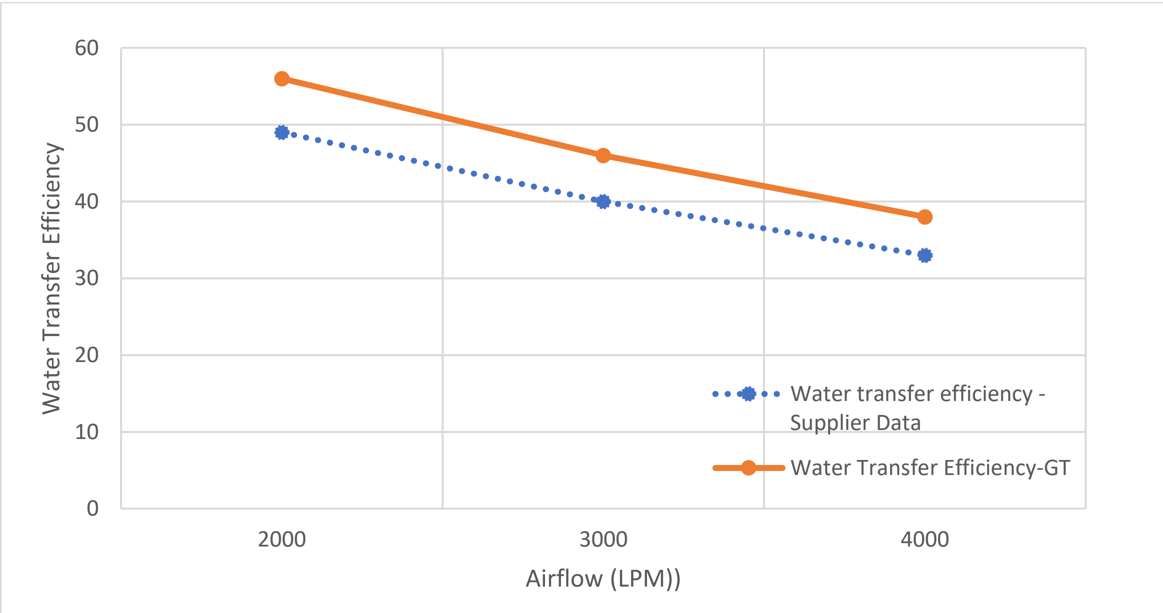

Fig 5. 25 Data Validation – Water transfer efficiency

From Fig 5. 24 it can be seen that a decent accuracy for the model is achieved. From Fig 5. 25 we see that the water transfer efficiency is higher in GT-suite. This may arise from the difference in the membrane modelling and the real membrane behaviour. Since there is no data for the behaviour of the membrane available, the default membrane provided by GT-Suite is used.

5.2.5 Fuel Cell Stack

Modelon Impact

A predefined template of the PEMFC stack is available in the component library, see Fig 5. 26. This template is parameterised by a Powercell intern and a colleague Mounir. It consists of a substack with connectors for feed and drain for the reaction gases for both anode and cathode. It consists of electrical pins for positive and negative and also a proton exchange membrane which is defined in a substack model. The model consists of pipe objects through which the coolant is passed and its respective connectors for feed and drain. The stack consists of a thermal connection (red line) between the substack and the cooling pipe which is used to maintain stack temperature. The stack consists of several substacks which are parameterised by the number of cells.

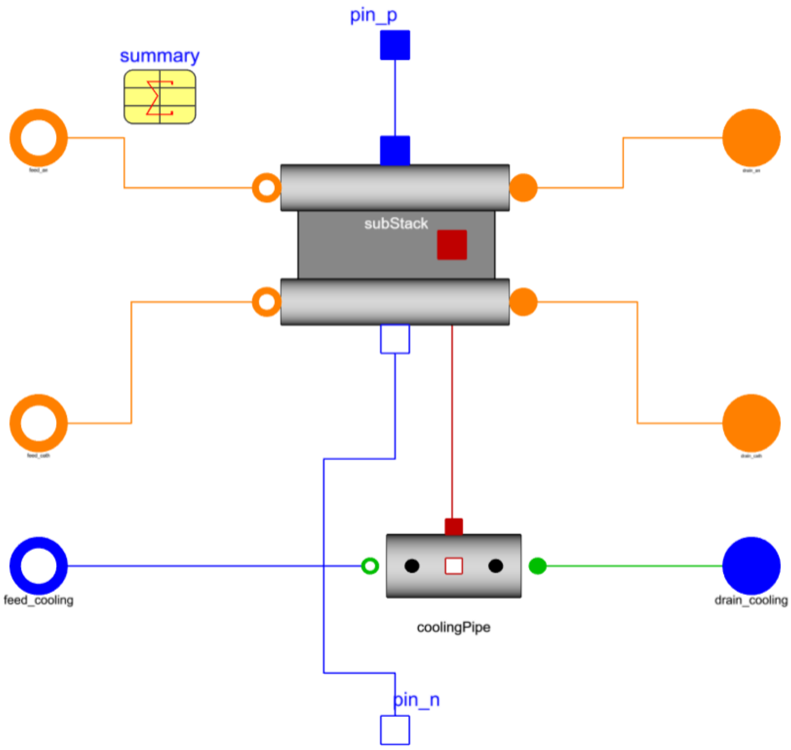

Fig 5. 26 PEMFC stack model with cooling

The substack (see Fig 5. 27) is used to illustrate a single cell which can be a lumped subset of the stack or a complete stack. The substack is defined by the membrane model and flow channels. The membrane model is a crucial component of the substack as all the electrochemical reactions and the mass and heat transfer between anode and cathode takes place here. The flow model is defined by the flow geometries, volume, flow direction, inlet pressure and temperature and mass fractions of the gases. The flow model additionally has heat flow connectors between membrane and anode and cathode channels through which the heat is transferred. Otherwise, there is no reaction occurring in the channels.[20]

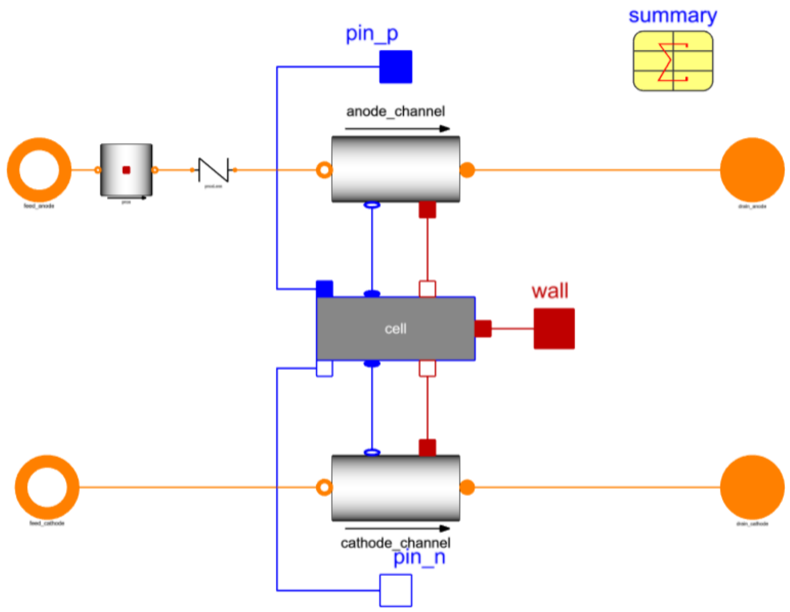

Fig 5. 27 Substack model with anode and cathode channels and cell membrane.

GT-Suite

A pre-existing template exists within the electrical library in GT-suite, see Fig 5. 28. This pre-existing template is parameterised by an intern and colleague Mounir and optimised to reflect the behaviour of Powercell stack. This template models a PEMFC's mass transfer, heat transfer, electrical power generation. The anode and cathode channels are modelled as pipe objects with pressure drop and friction connections. Similar to Modelon Impact, the channels are parameterized by their geometry and the initial states of the respective fluids. Hydrogen passes through the anode and similarly, air or oxygen passes through the cathode. On the exit side of both the channels, hydrogen and oxygen along with water vapour is removed on the cathode side. The water vapour arises on the cathode side inside of the fuel cell model following the chemical reaction and electron production to fit the current production. There are usually internal losses that cause the heat to be generated. The heat generated is transferred to the anode and cathode channels via the cell's thermal mass, also to the coolant and external environment as per the design or model of the fuel cell.[21]

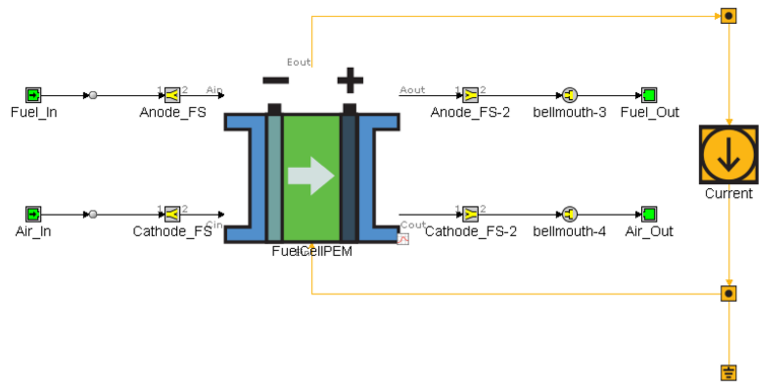

Fig 5. 28 Fuel Cell Model

6. Fuel Cell System modelling

Once the auxiliary components are modelled and validated with the supplier data, the components are integrated to form a working system around the fuel cell stack. This connection of components with a functioning fuel cell stack is termed as 'Fuel Cell System'.

Modelon Impact

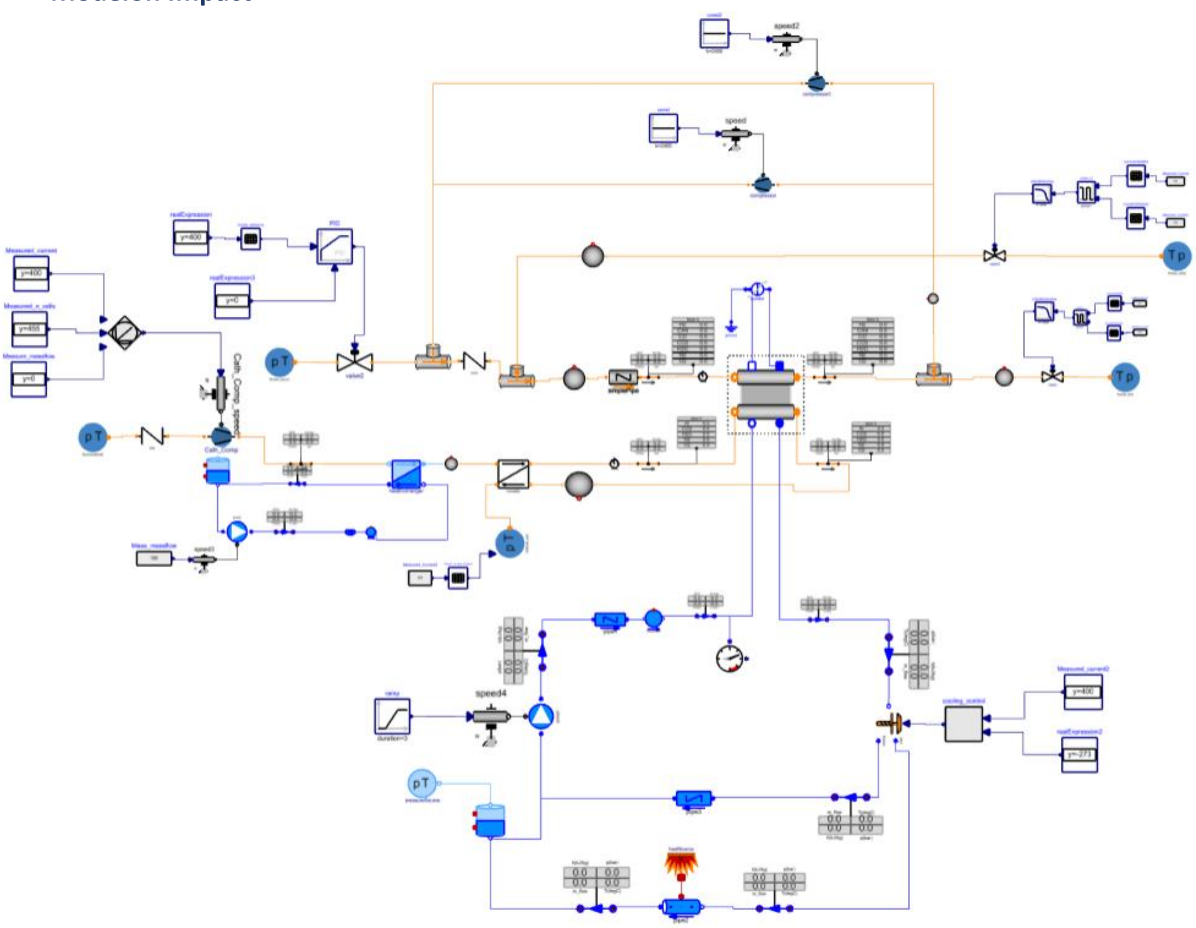

Fig 6. 1 Fuel Cell System Model in Modelon Impact

Error! Reference source not found. describes the modelled fuel cells system using all the components from its respective libraries. The blue streams towards the bottom of the model represent the cooling circuits. The gas streams are represented by the orange lines. The orange line loop in the top part of the stack represents the anode circuit. And the middle orange loop represents the cathode loop. The blue line from the top of the stack represents the electrical circuits.

GT-Suite

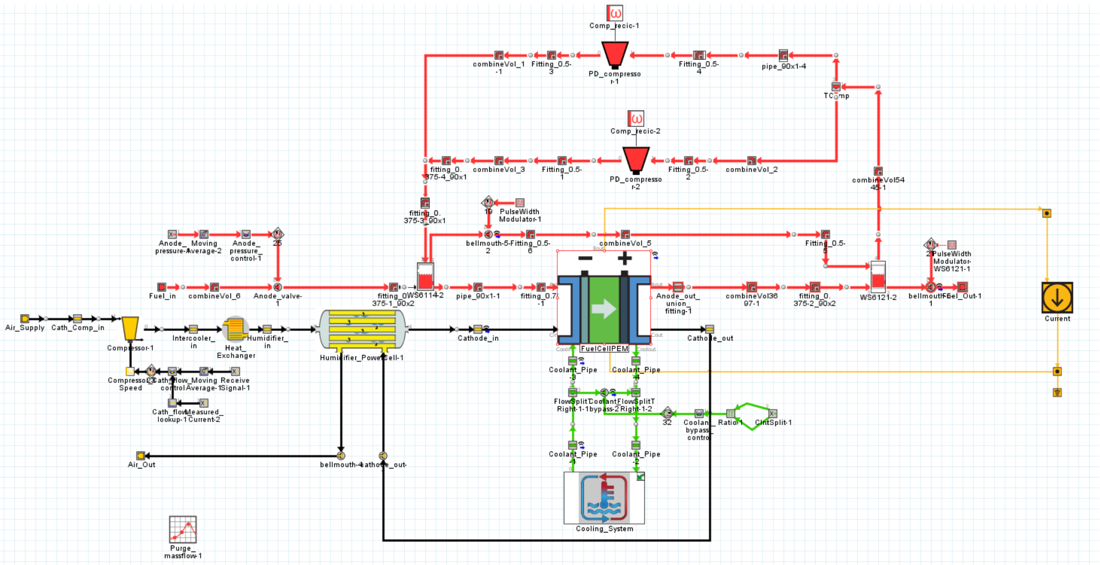

Fig 6. 2 Fuel cell system model in GT- Suite

Fig 6. 2 depicts, how the fuel cell system looks like when modelled with the respective components in GT-Suite. The red lines represent the anode flow system. The black lines represent the cathode flow system, and the green lines represent the cooling circuit. And the orange line is used to represent the electrical circuit.

6.1 Controls

Once the Fuel cell system is set up, it is usually set up to run at one particular condition. That means the components are connected, but they are not regulated to react to different operating conditions. For example: At a current of 100A, all the components have their respective working conditions. However, if one decides to run the system at 400A instead, the simulation will not proceed to give a result but will flash an error message. This occurs because, at 400A the demand for the reactants (H2, air) and coolant differ (in this case higher) as compared to 100A. To regulate the components in the system, a control system needs to be in place. A control system ensures a strategic method of control and thereby reducing human effort and errors.[22]

Modelon Impact

In Modelon Impact, a control strategy is implemented using PID controllers.[23]Lookup tables are used to control the set points of the controllers. The lookup tables are retrieved from actual system control data from Powercell. The controllers are used in four key places.

- One at the anode to control the hydrogen pressure in the stack.
- One at cathode compressor to control the airflow based on the current being drawn from the stack. This is done with the help of the PID controller, lookup table and the measured mass flow of air before stack (Fig 6. 3).
- One at the cooling valve to control the temperature of the stack. The cooling control utilizes a PID controller to control the valve opening. The setpoint to the controller is input with the knowledge of the measured current and a

lookup table to control the target. The measured temperature at the inlet of the stack is used as the input to the controller (Fig 6. 4).

- One at the anode exit to eject accumulated condensed liquid water and accumulated nitrogen. The control for the ejection uses a pulse input together with the lookup table to control the pulse for different currents (Fig 6. 5 Purge ControlFig 6. 5).

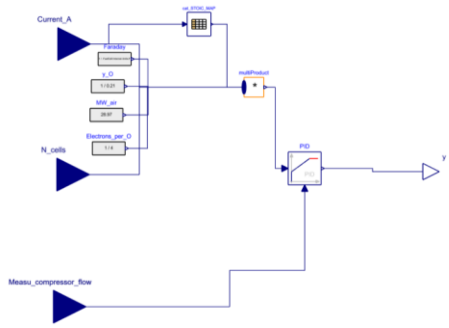

Fig 6. 3 Cathode Compressor Control

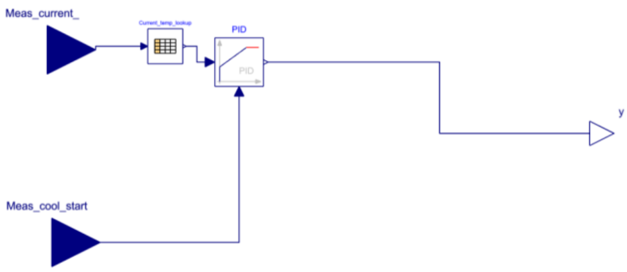

Fig 6. 4 Cooling control

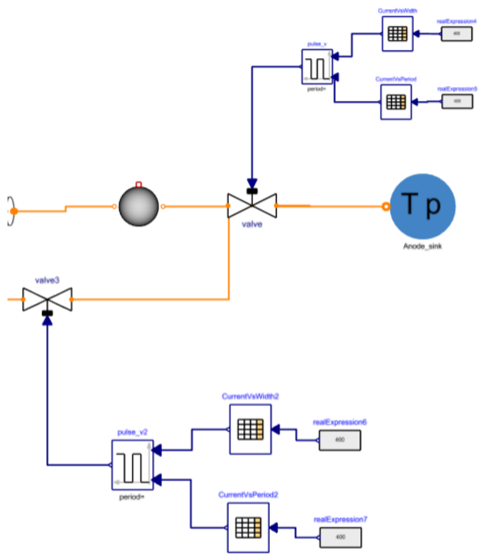

Fig 6. 5 Purge Control

GT-Suite

The same approach is used using GT-suite as well. The PID controllers are engaged to control the respective components. The difference between the modelling and simulation of the control strategy in Modelon Impact and GT-Suite is minimum to none. Some of the figures to depict the control is shown below. The contents of controls are provided by the active controls in the actual system and later fine-tuned in accordance with simulated result response. Fig 6. 6 to Fig 6. 9 describe four key controls in the system as depicted below.

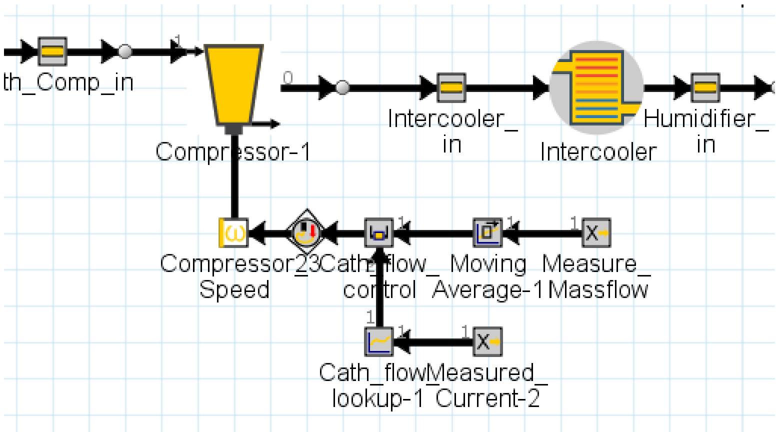

Fig 6. 6 Cathode Compressor Control

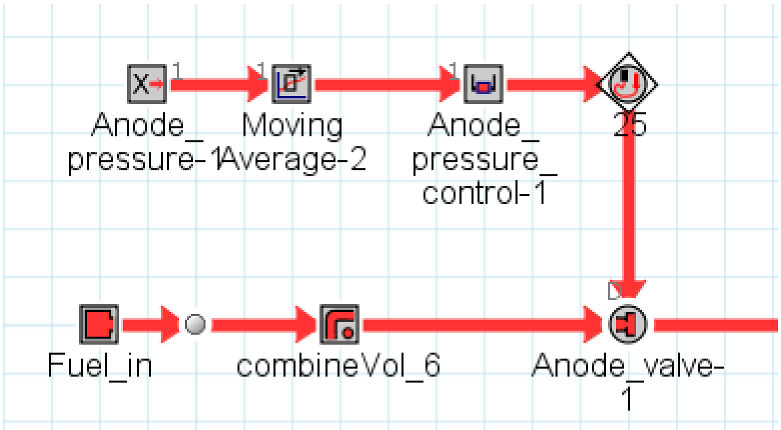

Fig 6. 7 Anode Pressure Control

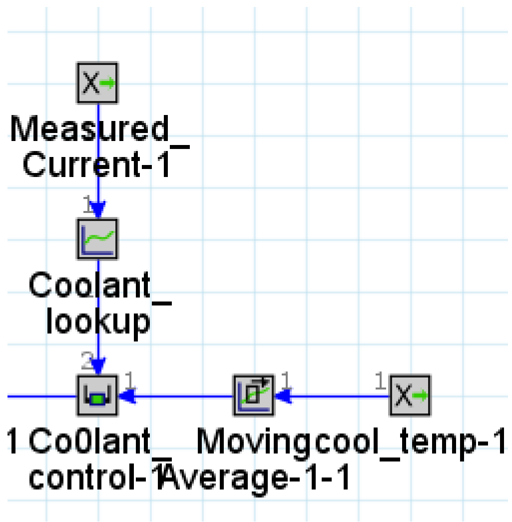

Fig 6. 8 Cooling Control

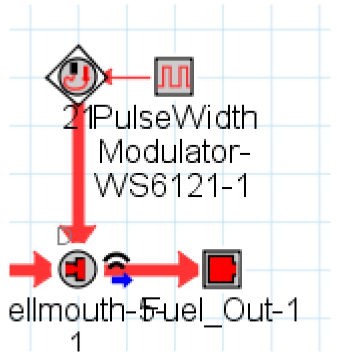

Fig 6. 9 Purge Control

6.2 Monitors and Post Processing

During the runtime of the simulation, the monitors help to visualise and understand the process better and help to improve the initialization of the system model. Monitoring also aids in understanding system behaviour at multiple locations or parts that are intricately connected in the model [22], for ex: pumps, bypass, controllers and compressors.

Modelon Impact

In Modelon Impact, the system variables are first visualized after the simulation is complete. Visualization can either be done by a so-called "sticky" showing the value as a function of time or a variable or by x-y diagrams. Furthermore, there are monitors available showing multiple properties of gas streams.

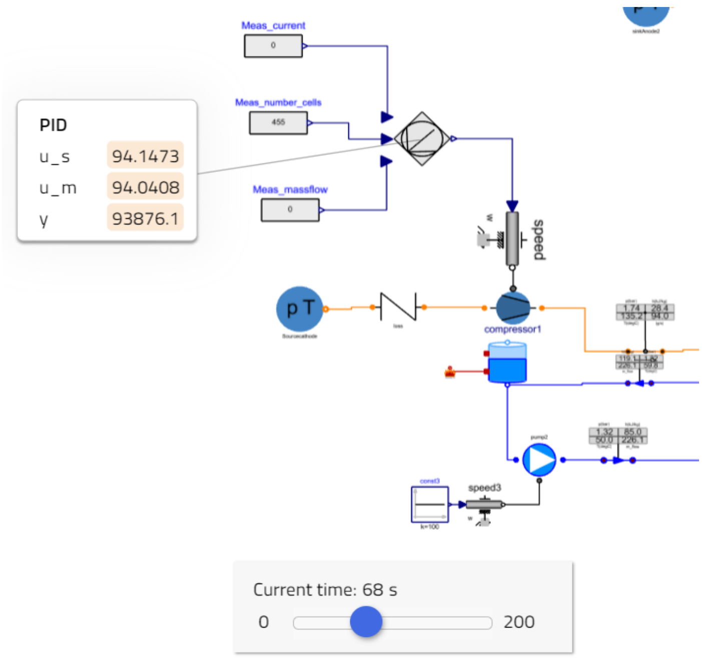

Fig 6. 10 Slider with changing characteristics of a controller numerically.

Fig 6. 10 describes the post-processing view with the help of a slider. In Fig 6.11 an example of the change in the characteristic of a controller is shown.

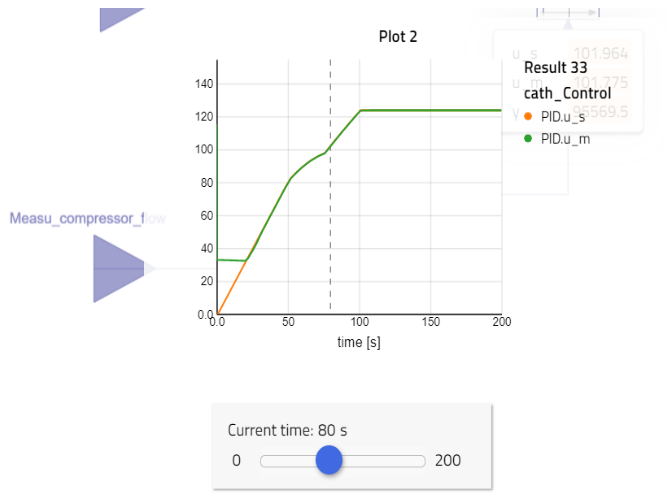

Fig 6. 11 Post-processing view of characteristics change graphically

Fig 6. 11 describes the same changes as seen in Fig 6. 10 but with a graphical template. If the simulation is halted midway to completion, the data is lost and cannot be viewed until the point of halt. This issue is however fixed in the upcoming updates of the software.

GT-Suite

In GT-Suite there are options to view monitors as a real-time view.

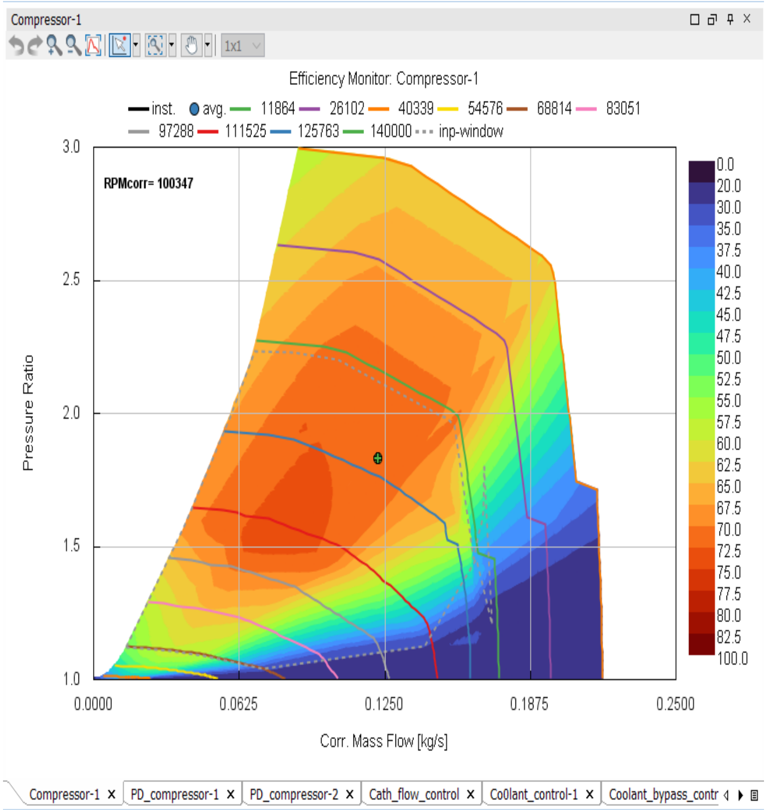

Fig 6. 12 Live view monitor of the cathode compressor.

Fig 6. 12 shows the real-time view of a compressor. The small green '+' shows at what point the compressor is operating. This gives a better understanding of the mapping of the compressor.

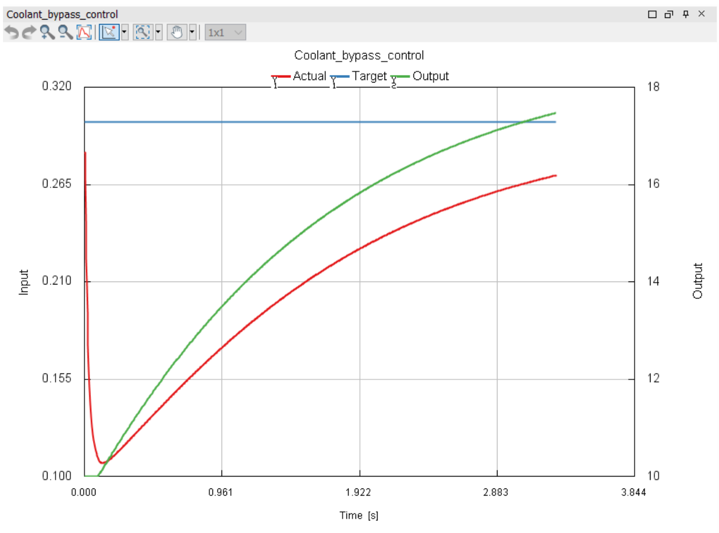

Fig 6. 13 Live view of response controller

Fig 6. 13 illustrates the live view of the controller which shows the response of the output of the controller to the delay in the actual response of the component.

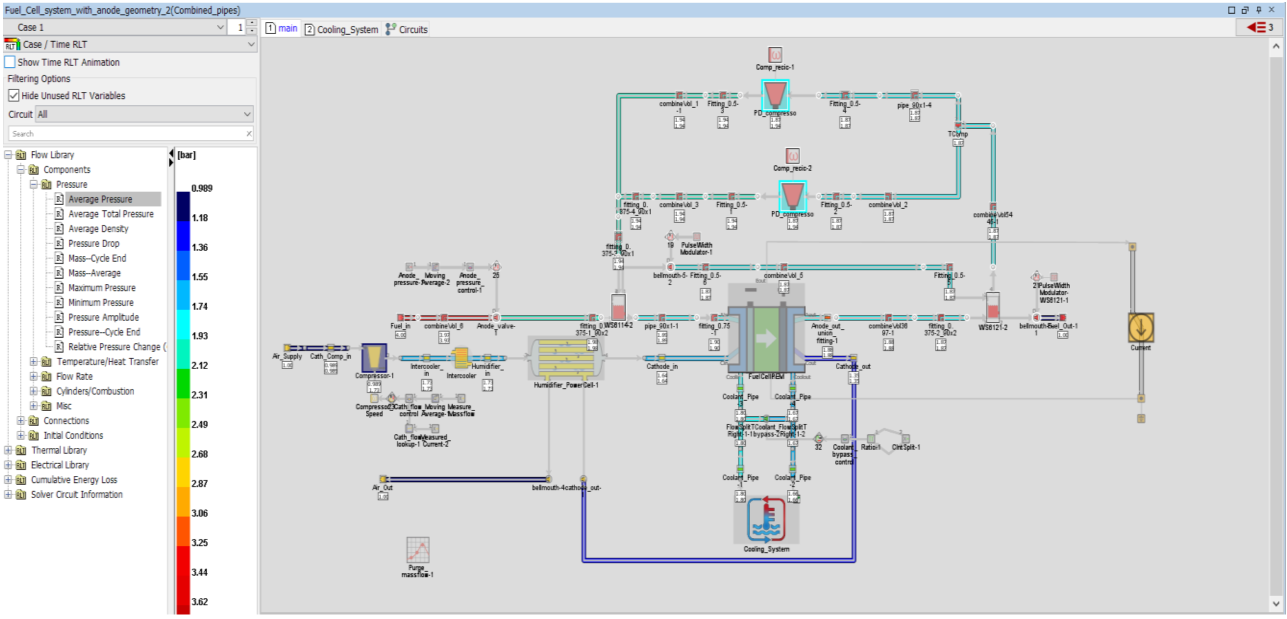

Fig 6. 14 Post-processing view GT-Suite

From Fig 6. 14 it can be seen that there are multiple parameters that can be viewed at the same time. If the focus is shifted to the left part of Fig 6. 14, it can be seen that there are multiple views. If average pressure is selected as in this case, the pressure across all the components and systems are visualised according to the colour scale. Similarly, temperature and flow rates can be viewed. This gives a broad overview of where one might enhance or tweak the design. This is a great advantage for simulation and modelling.

6.3 Additional detailing to flow circuits and pressure drop

For the improvement of the system model and simulation, the exact geometries of the flow channel were imported from CAD files to excel. The geometries and bends were incorporated into the anode system to check for and get closer results for the pressure drop in the system. A similar approach was done for cathode flow channels, but instead of importing the measurement data onto excel, a tool within GT-suite called GEM 3D and Spaceclaim was used. GEM 3D is a pre-processing tool that helps build and import 3D files and convert them to build 1D models.[24] The CAD file for the cathode system was imported in GEM 3D. From GEM 3D, the pipes with the bends and tapers were converted to 1D pipes. These pipes were then arranged in the right order of connections and simulated. This provides the right geometries and improves the pressure drop behaviour of the cathode system. The improved pressure drop is compared to the system pressure drop to get an idea of the accuracy of the modelling as can be seen in Fig 6. 15. There is some additional component detailing that hasn't been covered in the modelling due to the time frame of the thesis. This additional work has improved the system validation as can be seen in Fig 6. 17. The pressure drop modelling is done on the cathode and anode channels of the model in GT-Suite alone and not in Modelon Impact. To mimic the real system behaviour, the experimental piping pressure drop was assigned directly to the boundary condition. This explains the BOP consumption for Modelon Impact which matches better than that of GT-Suite.

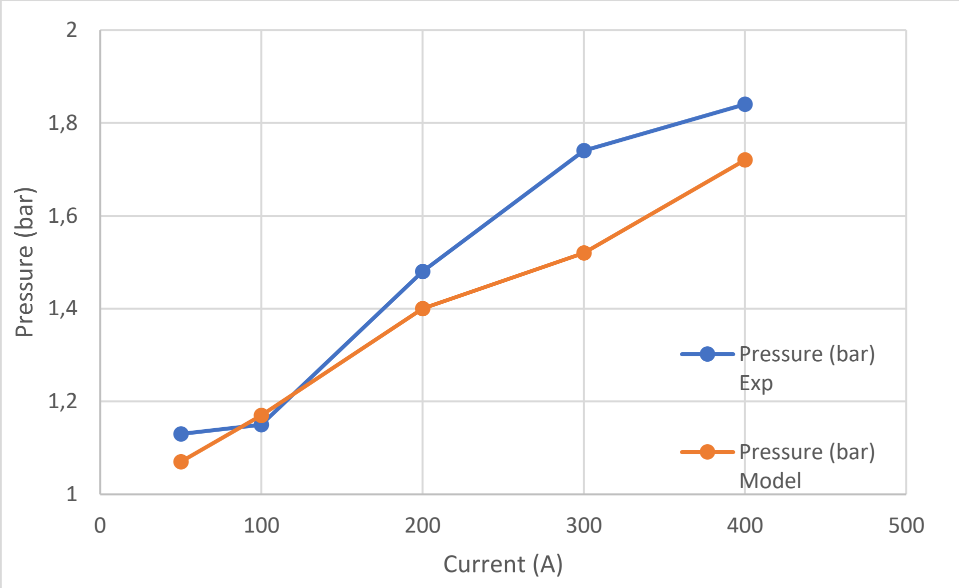

Fig 6. 15 Pressure drop comparison

6.4 System Validation

Once the entire process of modelling is carried out, the modelled data is compared to the data from the real system. The deviations and the similarities in the performance and the results become the basis for the selection of software. This also gives a decent outlook on if it can be used as a predictive model in the future. The validation is done on the basis of a performance graph which shows voltage, electrical power produced from the stack and the net power as a function of current. Net power is the system output power i.e. stack power subtracted by the power demand of the balance of plant components. The aspect to note here regarding the validation is that 100% accuracy cannot be achieved. The deviations may arise due to the level of detailing of system components for ex: stack with membrane and catalyst, humidifier etc.

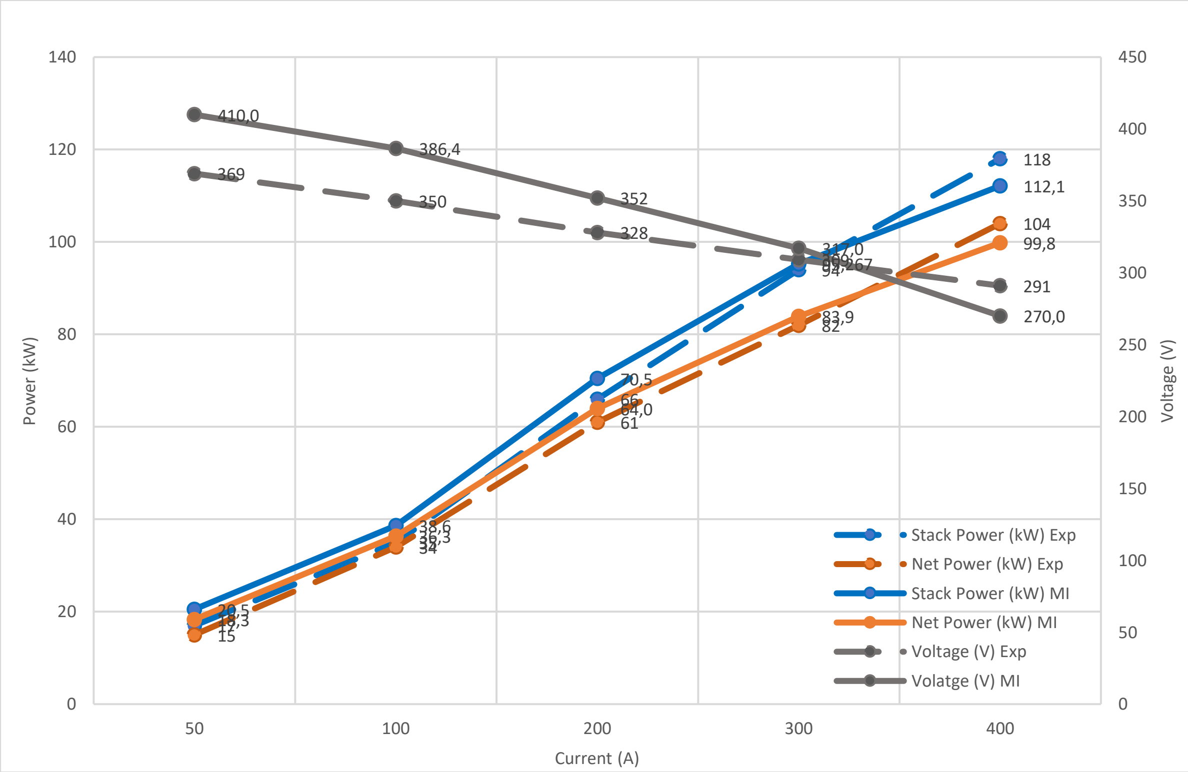

Fig 6. 16 Performance graph of the validation of Modelon Impact data with Experimental System data

Fig 6. 16 illustrates the similarities and deviations of the modelled data from Modelon Impact from the real system performance data. From the legends, 'Exp' depicts the experimental system data and 'Model' depicts the modelled data. The deviations in the voltage arise from the stack modelling and parameterization with the highest deviation of 41V at 50 A. The stack model assumes no condensation and is an empirical model. The deviations of stack power and net power are 5.9kW and 4.2kW respectively at 400A.

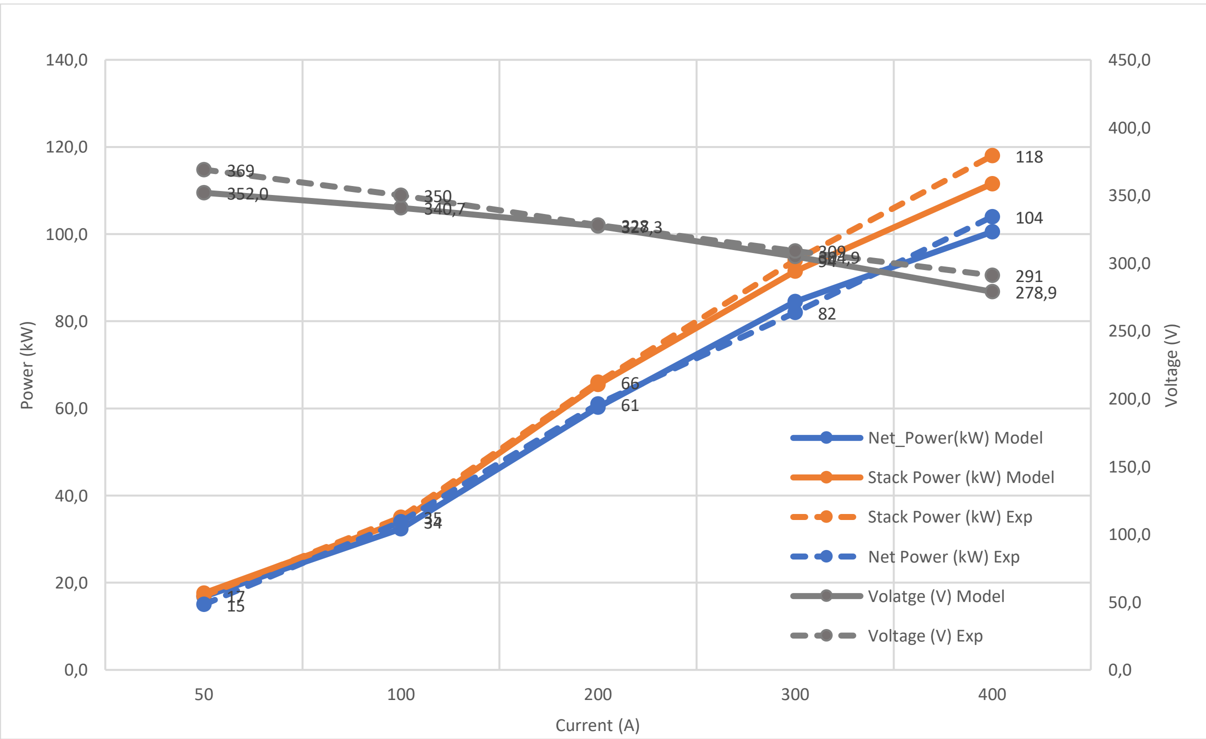

Fig 6. 17 Performance graph of validation of GT-Suite data with the system data

Fig 6. 17 illustrates the deviations and similarities of the GT-Suite modelled data and the experimental data. The highest deviation in the voltage is 17V at 50A and the highest deviations in stack power and net power are 6.4kW and 3.5kW respectively at 400A. This deviation in the higher current regions is due to the parameterization of the stack at higher current is not calibrated well enough.

As mentioned earlier, the net power is the power available from stack to use after the consumption of power from defined components of the system. Fig 6. 19 and Fig 6. 19 shows us the sum of power consumption at different current in the respective software. The comparison of actual system power consumption to the model power consumption is done and the match between them is fair. From Fig 6. 19 we can see a good match with slight deviations. The deviations at the lower current ranges may arise from the deviation from the controls of the compressor. The compressor is the most power-consuming component in the system. The deviation in the higher current may be due to the insufficient detailing of the pressure drops of the flow. From Fig 6. 19 we see a good match at 200A and below. For higher currents, power consumption is visibly lower in the model. This deviation can be explained with the scope of detailing of additional valves, filters and bypasses which exists in the real system but not in the model, see section 6.3 Additional detailing to flow circuits and pressure drop

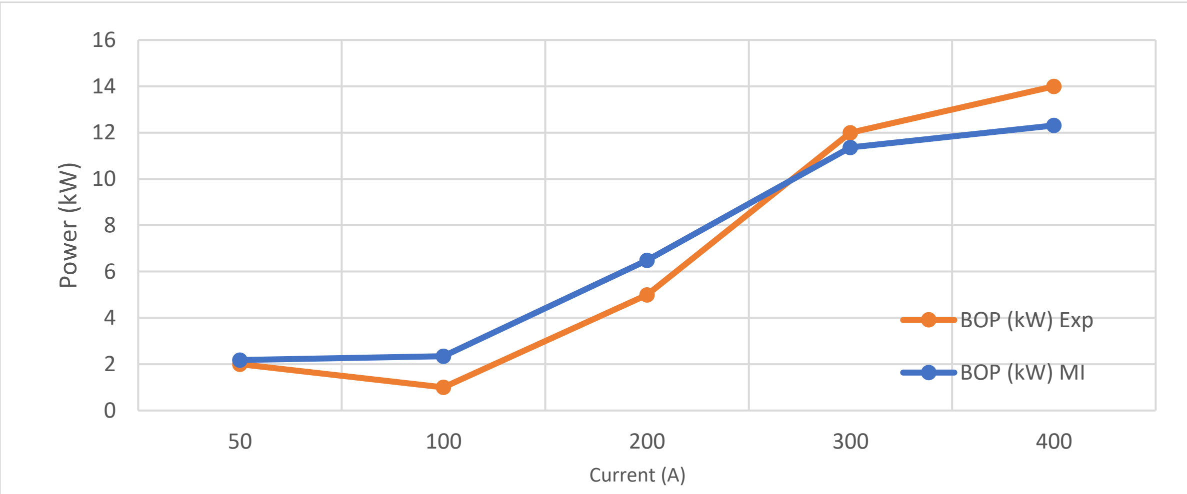

Fig 6. 18 Sum of Power consumption within the system (Modelon Impact)

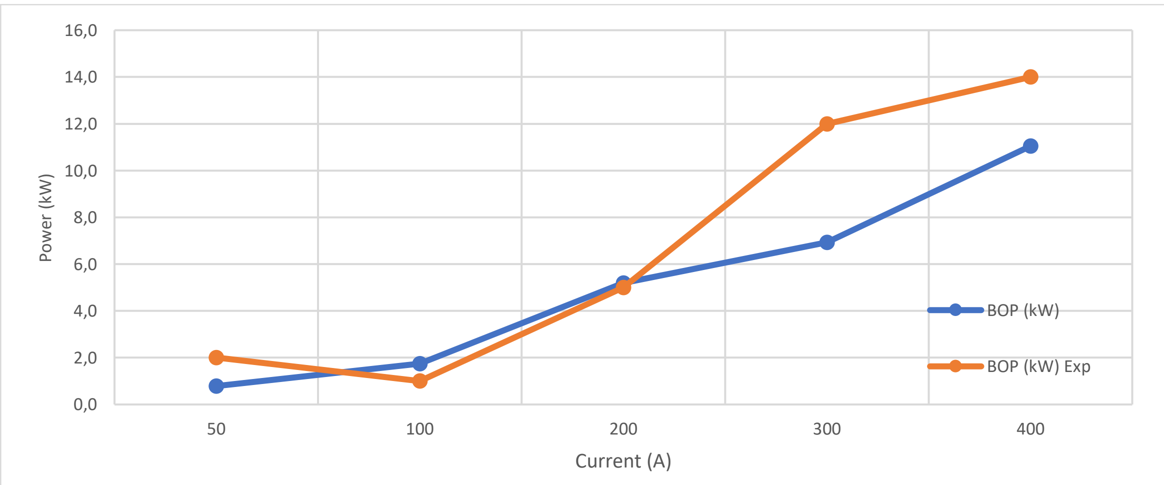

Fig 6. 19 Sum of Power consumption within the system (GT-Suite)

7. Conclusion

A 100 kW fuel cell system was modelled in both Modelon Impact and GT-suite. The described deviations in the individual models have a direct impact on the quality of the system model. It was shown that the maximum deviation of the net system power is 3.5 kW for GT-Suite and 4.2 kW for Modelon Impact (both for 400 A) The functionality of individual components is quite similar in both software except for the humidifier and the fuel cell stack. In the case of Modelon Impact, fully saturated gases are assumed in the humidifier which leads to the overprediction of the humidification. The humidifier model being beta, still has few bugs which have been reported to the software development team and will be solved in the coming updates. Since the updates and fixes are anticipated outside of the time frame of this thesis, a regular heat exchanger was used in place of the humidifier in the system model. The fuel cell stack is modelled in detail with GT-Suite as opposed to Modelon Impact with limited functionalities. This plays a crucial role as the stack voltage modelled in GT-Suite is much closer to the experimental voltage as compared to Modelon Impact (Fig 6. 16 and Fig 6. 17).

The workflow and ease of use with the components were quite similar with both software with additional points to GT-Suite to have unit conversions on the spot for the mapping of components. The effort required to efficiently map the components was a bit higher with Modelon Impact. Although, if this software is used quite vastly across different industries, the data handling units may get unified to fit the input for the software. Until then, it would be helpful to have a unit conversion for the ease of modelling a component. The workflow of the respective software was fairly simple with a drag and drop method. Modelon Impact has an interesting approach as to how a model is built in layers. The top layer is where one can input the information for the component. However, if one jumps down to the sublayer, a better understanding of the connections and the working of the component is discovered. This feature comes with a drawback with the complexity of the information that traverses to the top layer. This means, the sublayers are locked to any changes, and one must work with an isolated sublayer and refer this to the top layer. In the entire due course of this procedure, it may get confusing until one familiarizes with the workflow of the software. GEM 3D tool within GT- Suite provides the added benefit of importing the precise geometries which help to increase the detailing and level of accuracy of the model.

The documentation that guides and aids with the understanding of the working each component were on the same level of detailing in both the software. It is well explained and has easy access to the information required.

One advantage Modelon Impact has over GT-Suite is that its code is to a large extent open-source. This provides the advantage to people with a background in coding to exactly understand how a certain model is implemented and provides a platform to alter and tweak it to their convenience. This is however not possible with GT-suite, as it’s a pure GUI simulation software with the user limited to the exact functionality of the component as described in the respective documentation.

The technical support for both software was quite helpful. Contact information was available to persons to get in touch when facing specific problems. The response came within a single day which is impressive for both software.

After having worked with both software, a general impression is that the level of detailing for the component is higher in GT-Suite compared to Modelon Impact. GT-Suite provides the possibility to use data for the precise geometry of the component, ex: wheel diameter in a compressor and the type of membrane in a humidifier and its humidity transfer response along with thermal conductivity as a function of the flow of fluid etc. If the user does not have this precise data or chooses to ignore some of these parameters, it can be accommodated as well. With Modelon Impact the component template requires some data and it needs to be provided. There is no provision to enter additional data. It can however be implemented in the code layer, but not on the GUI. There is also no option provided to ignore certain variables of the component, unlike GT-Suite. Lastly, each software has its own advantages and disadvantages over the approach to its simulation structure. The user may have different needs and constraints before the selection of the software like the effort involved for modelling along with the intensity of use, the accuracy of the modelling and pricing of the software. The right trade-off of all this is finally in the hands of the consumer.

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