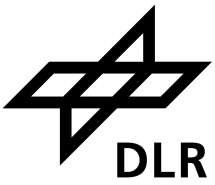

Development of PEM FCS model for Vehicle Digital Twin

Faculty of Electrical Engineering and Computer Science
Hochschule Ravensburg-Weingarten
Course of Study - "Master Mechatronics [M.Sc.]"

Master Thesis

in partial fulfilment of the requirement for the academic degree
Master Mechatronics [M.Sc.]

presented by

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Declaration

The Master Thesis titled 'Development of PEM FCS model for Vehicle Digital Twin' has been submitted as part of my Master degree program in Mechatronics at Hochschule Ravensburg-Weingarten. This work has been done in collaboration with "Deutsches Zentrum für Lüft- und Raumfahrt(DLR)" at the "Institute of Technical Thermodynamics".

I hereby declare that the content produced in this document is completely plagiarism-free. The information that is used from external resources is cited.

Stuttgart, 08 Feb 2024 David Venus Paul Inti

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Finally, I'm honored to have a supporting family, friends, and mentors who have always motivated me to go beyond my limitations.

Abstract

Proton exchange membrane (PEM) fuel cells are promising clean energy technologies because of their high power density and efficiency. However, developing efficient PEM fuel cell systems requires overcoming the challenges of multidomain complexities. Computer modelling and simulation helps by playing a crucial role in accelerating PEM fuel cell design and performance optimisation before moving to physical prototyping. One such tool is OpenModelica which is an open source modelling and simulation platform that supports multiphysics system modelling using Modelica's evolutionary and equation-based approach.

This thesis presents the development of a Proton Exchange Membrane (PEM) fuel cell system model using the OpenModelica open-source modelling platform. Individual cell components such as the membrane, catalyst layers and flow fields are modeled using circuit analogies and transport equations. The parameterized component models are assembled to build a modular fuel cell stack unit. This stack is supported by a Balance of Plant (BoP) that contains auxiliary subsystems such as Anode, Cathode and Coolant. The sensitivity analysis in the OpenModelica model is performed by evaluating the effects of demand inputs, such as fuel utilisation and temperature, on stack performance. Feedback control techniques such as PI control are applied to the system model to maximise power output while serving as a base for optimization of parameters and operation strategies.

The model is designed to be a base model, which can be equipped with different data from different manufacturers. This allows for efficient evaluation of design modifications and optimisation of model parameters for improved fuel cell performance and energy efficiency. The results obtained reveal that PEMFCS is able to accurately predict the desired voltage/power based on the demand input with a relatively low error. This model can be integrated into the Dymola environment along with existing vehicle models to act as a power source for a comprehensive analysis and testing.

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List of Abbreviations

PEMFC Proton Exchange Membrane Fuel Cell
PEM Proton Exchange Membrane
HOR Hydrogen Oxidation Reaction
ORR Oxygen Reduction Reaction
BoP Balance of Plant
SOFC Solid Oxide Fuel Cells
MCFC Molten Carbonate Fuel Cells
FCEV Fuel Cell Electric Vehicle
CL Catalyst Layer
GDL Gas Diffusion Layer
GDE Gas Diffusion Electrode
MEA Membrane Electrode Assembly
BP Bipolar Plate
DC Direct Current
AC Alternating Current
PI Proportional Integral
PID Proportional Integral Derivative
OM Open Modelica
RH Relative Humidity
H_2 Hydrogen
O_2 Oxygen

Nomenclature

V_{fc} - Fuel cell voltage (V)
R_{ohm} - Internal resistance (Ω)
i_{fc} - Fuel cell current (A)
E - Controlled voltage (V)
I_{net} - Net current (A)
Uf_{H2} - Hydrogen utilization
Uf_{O2} - Oxygen utilization
V_{act} - Activation voltage
E_{oc} - Open circuit voltage (V)
N - Number of cells
A - Tafel slope
i_o - Exchange current (A)
T_d - Response time (sec)
T - Absolute temperature (K)
P_{fuel} - Absolute supply pressure of fuel (atm)
P_{air} - Absolute supply pressure of air (atm)
V_{fuel} - Fuel flow rate (l/min)
V_{air} - Air flow rate (l/min)
x - Percentage of hydrogen in the fuel (%)
y - Percentage of oxygen in the oxidant (%)
P_{H2} - Partial pressure of hydrogen inside the stack (atm)
P_{O2} - Partial pressure of oxygen inside the stack (atm)
P_{H20} - Partial pressure of water vapor (atm)
E_n - Nernst potential (V)
w - Percentage of water vapor in the oxidant (%)
z - Number of moving electrons (z = 2)
α - Charge transfer coefficient
k - Boltzmann's constant (1.38×10-23 J/K)

h - Planck's constant (6.626×10-34 J s)

ΔG - Activation energy barrier (J)

K_c - Voltage constant at nominal condition of operation

1 Introduction

Fuel cells play a significant role in sustainable energy systems due to their high efficiency, low emissions, and versatility in various applications. According to [1] , fuel cells are electrochemical devices that directly convert the chemical energy of fuel into electricity, and they do not require recharging, making them a reliable and sustainable energy source. Ortiz Rivera[2] emphasizes the need for a new power source to address negative consequences of using fossil fuels, and highlights fuel cells as having the potential to meet the global power needs while meeting efficacy and environmental expectations. Furthermore, Spiegel[3] - outlines the advantages of using fuel cells in various sectors such as the portable sector, transportation market, and stationary sector, thereby contributing to the reduction of environmental emissions and providing cleaner energy solutions.

Furthermore, Ryan O'Hayre[4] mentions that fuel cells can be essential in reducing emissions by switching to fuels with low or zero levels of carbon and using more efficient energy conversion devices such as fuel cells.

The importance of accurate modeling and simulation in developing PEMFC systems lies in their ability to evaluate various design parameters and operating conditions to enhance performance and efficiency. Accurate models allow for the analysis of the transient response of PEMFCs, aiding in the identification of optimal design and real-time control for a wide range of applications, particularly in electric vehicle usage. Furthermore, these models help in studying the system's dynamic and steady-state behavior, enabling the assessment of different flow channel designs and their impact on reactant distribution, proton conductivity, and thermal management. Such thorough analysis supports the identification of key optimization parameters for performance improvements in PEMFC systems.

1.1 Background

The historical evolution of PEMFCs has been significant in shaping the landscape of renewable energy technologies.

The dependency on fossil fuels as a primary energy source has driven the search for suitable renewable substitutes. Hydrogen technology, expected to play a crucial role in meeting energy and carbon saving criteria, has gained importance, with advanced hydrogen technologies like fuel cells creating new business opportunities [5]. Specifically, PEMFCs have emerged as a promising candidate for future energy systems, notably for portable, transport, and stationary applications [5]. Over the years, consistent improvements in single cells, fuel cell stacks, and complete systems have paved the way for prototype mobile applications, fuel-cell powered demonstration vehicles, and field tests of combined heat and power units in various countries [5].

In the context of renewable energy, PEMFCs have gained attention due to their high energy density, high conversion efficiency, low operating temperature, and low gas emissions. Their potential as an alternate source for automotive mobility, with zero carbon emissions, adds to their significance in the renewable energy landscape, aligning with efforts to reduce emissions from transportation [6]. Drawing on this historical evolution and significance, the advancements in PEMFC technology contribute to the global transition towards cleaner, reliable, and sustainable energy systems.

The research and development of PEMFCs are propelled by pressing environmental and economic imperatives. From an environmental perspective, the attributes of PEMFCs, such as low operating temperatures and minimal pollution, align with the global efforts toward sustainable and eco-friendly energy solutions [7]. The potential of hydrogen-based technologies, including fuel cells, to reduce carbon emissions and mitigate environmental impact is a driving force in the development of PEMFCs [6]. Furthermore, the advancement of PEMFC technology has the capacity to contribute significantly to the reduction of greenhouse gas emissions in various applications, such as automotive transportation and stationary power generation [6] [5].

On an economic front, the growing demand for cleaner energy technologies has led to substantial investments and incentives in the development and commercialization of

PEMFC systems. The potential market expansion for fuel cell technologies, driven by environmental regulations and policies, has created significant economic opportunities within the renewable energy sector, stimulating economic growth and job creation [6]. Additionally, the promise of enhanced energy efficiency and reduced reliance on conventional energy sources further fuels the economic motivations for PEMFC research and development [6].

The convergence of these environmental and economic factors underscores the significance of PEMFCs in the transition toward sustainable and efficient energy technologies.

Table 1.1 displays the primary operational principles and operating temperatures of several fuel cell types.

Type of Fuel Cell	**Fuel**	**Membrane**	**Oxidation Agent**	**Operational Temperature (°C)**
Solid Oxide Fuel Cell [8]	H_2, CO	Ionconducting ceramic	O_2	1000
Carbonate Fuel cell [9]	H_2	Molten Alkaline melt	O_2, CO_2	650
Phosphoric Acid Fuel cell [10]	H_2	Phosphoric acid	O_2	200
Direct Methanol Fuel Cell [11]	CH_3OH	Ionconducting polymer	O_2	80–110
Proton Exchange Membrane Fuel Cell [12]	H_2	Ionconducting polymer	O_2	65–85
Alkaline Fuel Cell [13]	H_2	Caustic potash	O_2	20–90

Table 1.1: Comparison of different types of fuel cells.

1.2 Principle of operation of PEMFC

The principle of operation of a PEM fuel cell involves the electrochemical reaction between hydrogen and oxygen to produce electricity. The fuel cell consists of an anode and a cathode separated by a proton exchange membrane. At the anode, hydrogen molecules are split into protons and electrons. The protons pass through the membrane, while the electrons flow through an external circuit, creating an electric current. At the cathode, oxygen molecules combine with the protons and electrons to form water. This reaction occurs in the presence of a catalyst, typically platinum, which facilitates the movement of protons and electrons. The overall efficiency and voltage output of the fuel cell depend on factors such as thermodynamic behavior, polarization analysis, and concentration of reactants[14].

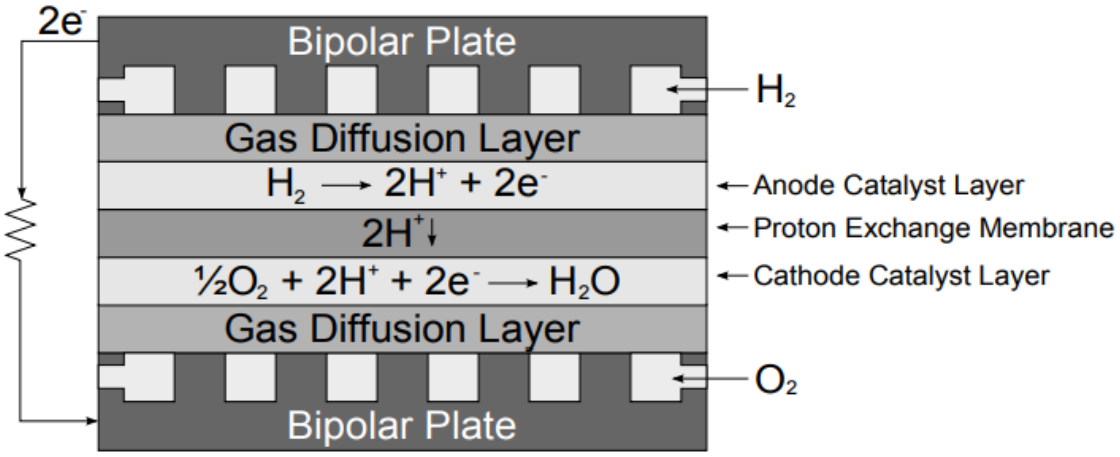


Figure 1.1: PEMFC Schematic

In a PEMFC, the fundamental electrochemical reactions that occur are the hydrogen oxidation reaction (HOR) at the anode and the oxygen reduction reaction (ORR) at the cathode.
The hydrogen oxidation reaction occurs at the anode, where hydrogen molecules are split into protons and electrons as represented by the equation 1.1:

$$\mathrm{H_2} \longrightarrow 2\,\mathrm{H^+} + 2\,\mathrm{e^-} \tag{1.1}$$

The oxygen reduction reaction takes place at the cathode, where oxygen molecules combine with protons and electrons to form water as shown by the equation 1.2:

$$\frac{1}{2}\,\mathrm{O_2} + 2\,\mathrm{H^+} + 2\,\mathrm{e^-} \longrightarrow \mathrm{H_2O} \tag{1.2}$$

These reactions are pivotal in the generation of electrical energy within a PEMFC and are central to the overall operation and performance of the fuel cell as shown in fig 1.1[15].

The graph shown in fig 1.2 is a general polarisation curve for a PEMFC. This graph illustrates the correlation between the voltage output of the fuel cell and the current density, which quantifies the amount of current generated per unit area of the cell. The curve is conventionally partitioned into three discrete areas, denoted as i, ii, and iii, each representing separate physical events occurring within the fuel cell:

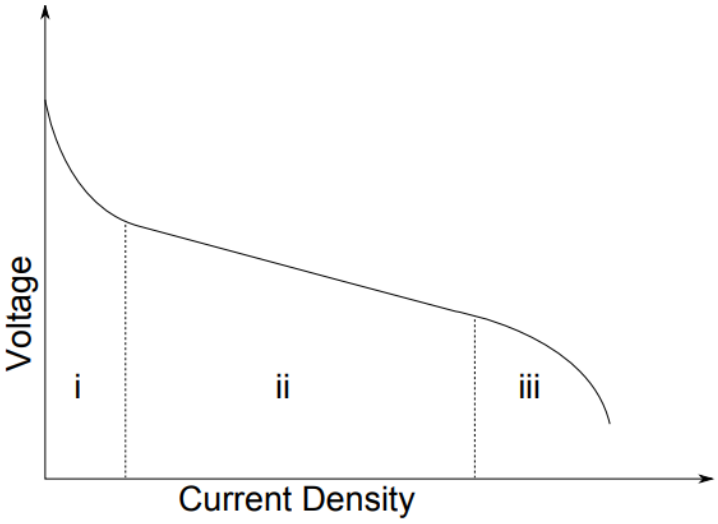


Figure 1.2: General polarization curve loss regions: (i) activation, (ii) ohmic, and (iii) concentration.

Region i: Activation Polarization

This region corresponds to the first part of the curve, characterised by a rapid decrease in voltage as the current density increases. The main reason for the high slope in this area is mostly attributed to activation losses, which are associated with the amount of energy needed for the electrochemical reactions to occur at both the anode and cathode. The magnitude of these losses is particularly notable while operating at low current densities, as the overpotential needed to surpass the activation energy barrier is at its maximum. The fuel cell's efficiency is at its peak at the start of this range, but decreases rapidly as the current density rises.

Region ii: Ohmic Polarization

This section represents the middle part of the curve, where there is a gradual decline in voltage as the current density increases. The losses in this particular area are a result of the internal resistance shown by the various components of the fuel cell, including the electrolyte, electrodes, and the contact resistances between these components. This is

the point at which ohmic losses, also known as resistive losses, are the most significant. These losses remain consistent throughout this range of current densities and result in a corresponding decrease in voltage as current rises.

Region iii: Concentration Polarization

This is the final segment of the curve, characterised by a steeper decrease in voltage. The significant decline is attributed to the losses in concentration. As the current density escalates, the pace of the electrochemical processes also intensifies. This can lead to a rapid reduction in the availability of reactants at the reaction sites, surpassing their rate of replenishment through diffusion, resulting in a decline in voltage. When subjected to high current densities, the fuel cell's capacity to generate high power output is hindered by the restricted supply of reactants, resulting in a significant decrease in efficiency.

1.3 Research objectives

Main Objective:

The primary aim of this research is to build a simple, yet effective, time-dependent model of a PEMFC system that can be easily integrated into vehicle simulations. The focus is on capturing the dynamic responses of the fuel cell stack and the BoP in a way that's both efficient and practical for simulation purposes.

Secondary objectives:

- The model will be designed to be straightforward and quick in computation, making it an ideal foundation for future real-time simulations, especially for complex vehicle simulation environments.
- A key aspect of this model is its modular structure, allowing for easy adaptation and expansion in subsequent research phases.
- The model should have the capacity to adjust and include diverse data from various manufacturers in order to demonstrate its practical usefulness in rapid

assessment and facilitate incremental improvements to its design.

This thesis further explores these issues by utilising OpenModelica to construct an intricate model of a PEMFC system. The methodology integrates modelling at the component level and simulations at the system level to enhance the design and optimise operating strategies, ultimately enhancing performance and efficiency prior to the construction of physical prototypes.

The development of this model will be conducted using OpenModelica, a strategic choice due to its compatibility with future vehicle models, its open-source nature, and the absence of licensing constraints. This makes OpenModelica an ideal platform for developing versatile and adaptable simulation models. The selection of OpenModelica is influenced by its potential for future integration with various vehicle models, underscoring its adaptability and relevance in the evolving field of vehicle simulation.

The research is driven by the need to enhance the application of PEMFC systems in vehicles, focusing on creating a model that is both user-friendly and robust enough to handle the complexities of real-world scenarios. The approach is grounded in practicality, with an emphasis on creating a model that can evolve over time and contribute meaningfully to the field of fuel cell technology in automotive applications.

2 PEM Fuel Cell Systems and Components: Insights

2.1 Motivation

Evaluating the efficiency of PEMFC requires conducting accurate experiments in a range of controlled conditions. This process often entails not only the careful assembly and building of the cell, but also the provision and secure handling of reactants. The use of operational equipment, including compressors, humidifiers, and sophisticated data collecting systems, is of utmost importance. Although a fuel cell test stand provides a complete control station, it is frequently excessively costly, requiring substantial laboratory resources and specialised expertise. The physical evaluation method is demanding, necessitating substantial effort to examine a wide range of design variables, including membrane selection, catalyst loading, and operational parameters such as temperature and pressure.

Preemptive computer modelling is highly helpful for streamlining the design and optimisation of PEMFCs. It allows for the prediction of cell performance without the necessity for expensive fabrication and testing. Modelling and simulation are powerful techniques that significantly reduce the financial and time costs usually involved in empirical testing. An accurate and extensively tested computer model can quickly assess several ideas with minimal additional expenses. Therefore, the accuracy of the model becomes a crucial factor in selecting a method to predict and improve fuel cell efficiency.

Furthermore, including numerical simulations into the research and development process enables the investigation of novel material options and structural arrangements. Incorporating this strategic element not only reduces risks but also speeds up the iterative process of enhancing design. Advanced computer simulations, such as those

conducted using platforms like OpenModelica, allow for thorough examination of fuel cell dynamics across a wide range of conditions. This is advantageous because replicating these conditions in a physical laboratory would be unfeasible due to logistical and cost limitations.

These simulations are not simply a replacement for experimental approaches, but rather a revolutionary methodology that fundamentally changes the direction of PEMFC research. This thesis presents a comprehensive OpenModelica model that offers a flexible framework for hypothesis testing, system behaviour validation, and control strategy optimisation. The model's versatility in integrating data from different manufacturers renders it an indispensable resource for predictive research and comprehensive comprehension of the fuel cell's operational intricacies. The simulation data obtained will provide valuable foresight into the feasibility of proposed design modifications, serving as a crucial tool for advancing PEMFC technology and optimising energy systems globally.

2.2 Literature Review

Prior studies on the modelling and simulation of PEMFC have yielded valuable insights in various crucial domains:

In the research conducted by Abd El Monem et al. [16], a simplified mathematical model for PEMFC systems was created and verified by comparing it to experimental data obtained from a commercially available PEMFC stack. The model effectively depicts the dynamic and steady-state characteristics of the fuel cell when subjected to various load fluctuations, showcasing the rapid response capabilities of the PEMFC in adapting to load changes.

The study also highlighted the significance of creating diagnostic and prognostic tools using the fuel cell system model to assess and enhance performance in terms of dependability and durability. The research conducted by Loic Vichard, Nadia Yousfi Steiner, and Daniel Hissel [17] emphasised the necessity for dependable diagnostic and prognostic instruments grounded in the fuel cell system model, taking into account various configurations and energy management strategies.

The current methods for dynamic modelling of PEMFC systems can be categorised into three groups: physics-based models, data-driven models, and hybrid models [17]. Physics-based models utilise system physical equations and possess strong generalisation capabilities, whereas data-driven models are constructed using measurable data and are sometimes regarded as black box models. Hybrid models integrate both physics-based and data-driven models.

Dynamic modelling of PEMFC systems is crucial for accurately reproducing the behaviour of the entire system, particularly in electric vehicle applications. The need of dynamic modelling in accurately representing the fuel cell's transient dynamics, particularly during acceleration and deceleration in electric vehicle applications, was underscored.

These findings offer useful knowledge on the creation and verification of PEMFC models, the significance of diagnostic and prognostic tools, and the classification of modelling methodologies. To gain a thorough understanding of PEMFC modelling and simulation, it is advisable to review the in-depth findings and analysis presented in [16] and [17].

Prior research has also established various modelling methodologies and instruments for PEMFC in the context of electric vehicle utilisation. The categorization of modelling techniques encompasses physics-based models, data-driven models, and hybrid models. Physics-based models utilise the physical equations of the system and provide strong generalisation capabilities, providing insights into the internal physical parameters. Nevertheless, a profound comprehension of the system's behaviour and degradation laws, along with familiarity with internal system information, is necessary.

Data-driven models, such as those utilising artificial neural networks, have the benefit of not needing internal system parameter information and not necessitating a thorough comprehension of system degradation laws. Nevertheless, these models require a substantial quantity of data for constructing and possess limited capacity for generalisation. Previous research has employed empirical, statistical, or mathematical models, such as machine learning algorithms and comparable circuit models.

Hybrid models aim to integrate the benefits of both physics-based and data-driven approaches. Although these models potentially provide a combined approach, there are currently only a limited number of published PEMFC hybrid models accessible. Hybrid models strive to replicate the dynamic behaviour of the system under consideration by combining physical and data-driven components. In order to thoroughly compare the many modelling approaches and tools that have been previously utilised, it would be essential to conduct a comprehensive review of their respective benefits, constraints, and specialised uses.

OpenModelica is an essential component of the Virtual-FCS project, as it functions as a cost-free and openly accessible modelling platform for simulating intricate dynamic systems, including PEMFCs. The software utilises the Modelica language, which leverages an object-oriented structure and acausal modelling method to construct a bond graph representation of a physical system [18].

OpenModelica is in accordance with the precise criteria outlined for the modelling environment of the Virtual-FCS project, as stated on page 10 in [18]. The software satisfies the requirements of being open-source, free, easy to use, modular, effective in solving interconnected non-linear equations, and capable of supporting hardware input/output. OpenModelica distinguishes itself from other simulation environments by offering capabilities such as hierarchical modelling, acausal equation formulations, and real-time system simulation support. In addition, the use of hardware-in-the-loop testing and synchronous real-time modelling in OpenModelica showcases its appropriateness for achieving the project's goals.

2.3 Overview of fuel cell technology

Fuel cell technology represents an innovative and promising approach to electrochemical energy conversion with diverse practical applications. Fuel cells directly convert the chemical energy of fuel into electricity and heat, offering numerous advantages over traditional power sources. These advantages include high efficiency, mechanical simplicity, modularity, low noise, and minimal environmental impact, particularly in terms of air pollution and greenhouse gas emissions. The scenarios where fuel cells are used encompass industrial, commercial, transportation, and residential construction sectors, demonstrating the versatility and potential of this technology.

The fuel cell landscape includes various types of fuel cells, such as the PEM fuel cell, which is considered a promising candidate for numerous applications due to its efficiency and environmental benignity. Other fuel cell types like SOFC and MCFC have also demonstrated their capabilities, each offering distinct advantages and suitable applications.

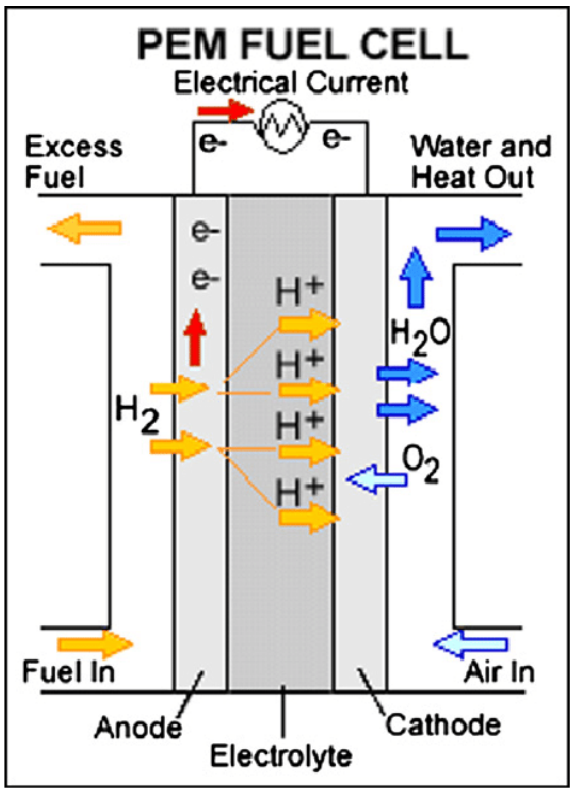


Figure 2.1: PEM Fuel Cell

In the context of transportation, fuel cells are being developed for use in FCEVs, with major automotive manufacturers investing in their development. Commercial success and advancements in FCEVs are evident through the market presence of notable models like Hyundai Nexo, SAIC Maxus FCV80, Honda FCX Clarity, and Toyota Mirai, each presenting key performance parameters.

The potential impact of fuel cell technology spans into diverse areas, including portable devices, transportation, and stationary power generation. For instance, in the portable

sector, fuel cells are envisioned to power various devices such as laptops, cell phones, and military equipment, offering extended power and improved efficiency.

While fuel cells offer a range of advantages, they also pose certain challenges and limitations. The high cost of materials, such as platinum catalysts used in PEMFCs, is a significant constraint, as is fuel cell power density compared to other power sources. Additionally, issues such as fuel availability and storage, as well as technology costs and power density, are among the limitations currently associated with fuel cell technology. Overcoming these challenges and further advancing fuel cell technology could lead to significant environmental and energy-related benefits, including reduced emissions and improved energy efficiency.

The operation of a fuel cell is primarily based on electrochemical processes, where reactions take place at the interfaces between the electrodes and electrolyte. These reactions involve the transfer of charge (electrons) between the electrodes and chemical species. The pace of power generation in fuel cells is influenced by the production and consumption of charge through electrochemical half reactions.

Fuel cell technology has attracted attention for its potential to significantly reduce environmental impact by offering low or zero emissions. This is particularly true when pure hydrogen is used as the fuel source, leading to decreased air pollution and greenhouse gas emissions. Nevertheless, the environmental consequences can be affected by factors such as the techniques used for hydrogen production and the total emissions throughout the lifespan of fuel cell systems.

The cost and maintenance of fuel cells are affected by various factors, including the high cost of platinum catalysts used in certain types of fuel cells, the expenses connected with the materials used, and the maintenance needs related to additional components and system design. Moreover, continuous progress and enhancements in materials and manufacturing techniques are aiding in cost reduction and enhancing the longevity and upkeep of fuel cell systems.

Fuel cells have several benefits, including as their superior power density, rapid start-up abilities, ability to operate at low temperatures, flexibility in fuel choices, and little maintenance requirements due to the lack of moving components. However, there are

some significant drawbacks that hinder the broad use and cost-effectiveness of fuel cell technology. These include the expensive platinum catalysts, costly components, the need for active water management, and the limited ability to tolerate specific impurities.

2.4 Fuel Cell Components

PEM fuel cells, which are renowned for their high energy efficiency and clean energy output, are made up of a number of essential components, each of which plays an important part in the operation of the cell. For the purpose of knowing the operation of PEM fuel cells and the prospective applications of these cells, it is vital to have a solid understanding of the structure and function of these components. Major components of a stack assembly are shown in fig 2.2 [19]

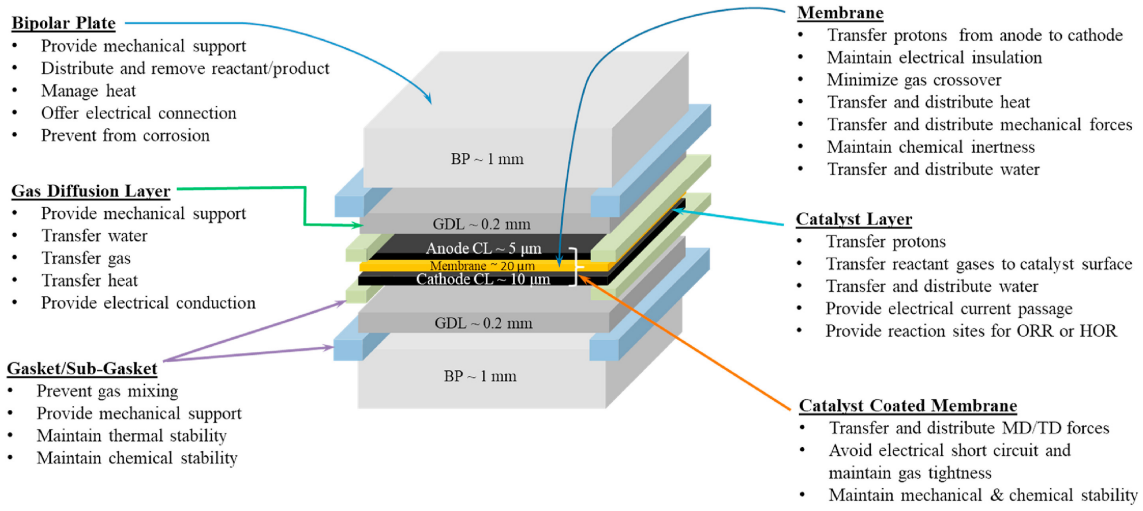


Figure 2.2: PEMFC Stack

2.4.1 Proton Exchange Membrane

The proton exchange membrane, which serves as a polymer electrolyte, is a crucial component of a PEM fuel cell. The proton-conducting polymeric membrane, which repels electrons, allows the electrons to flow through the external circuit, generating electrical work. The membrane's protonic conductivity can be increased by a higher concentration of fixed charges. which are being created as environmentally friendly and highly efficient energy sources for various sizes of applications, such as automotive and portable power. The Nafion perfluorosulfonic acid membrane, developed by DuPont, has been widely utilised in PEM materials because to its exceptional chemical and physical durability, as well as its superior proton conductivity. Nevertheless, there are a few disadvantages associated with it, including its high price, susceptibility to

methanol leakage, and restricted operational temperature range in fuel cells [20].A PEM is a crucial element of a PEMFC system. From a practical standpoint, an ideal PEM must satisfy the following criteria:

- Affordable.
- Minimal ionic resistance (i.e., high proton conductivity) during fuel cell operation.
- Strong mechanical properties, preferably with resistance to swelling.
- The capacity to maintain its chemical and mechanical properties for extended periods at high temperatures in both oxidising and reducing conditions.
- Minimal or no leakage of fuel or oxygen.
- Compatibility with catalyst layers.
- Electrical insulation.

2.4.2 Catalyst layer

PEMFCs have garnered significant interest due to their suitability for transportation systems and portable electronic devices [21]. The CL's present significant problems in PEMFC research due to their intricate and heterogeneous nature. The catalyst layers must be engineered to optimise the rates of the desired reactions while minimising the catalyst quantity needed to achieve the appropriate power output levels. In order to achieve the objective, it is necessary to take into account the following prerequisites:

- a substantial three-phase boundary in the cathode layer
- effective proton transportation
- convenient movement of reactant and product gases as well as elimination of condensed water, and
- uninterrupted flow of electronic current between the reaction sites and the current collector

A CL with a thickness of several micrometres is an essential element of a proton exchange membrane fuel cell (PEMFC) and necessitates more intricate processing [22]. The CL is in direct physical contact with both the membrane and the GDL, as seen in Fig 2.3[23]. The active layer is also known as [24]. Gottesfeld and Zawodzinski provide a comprehensive examination of the structure and functionalities of the CL [25]. Identifying the electrode structures and operation circumstances is crucial for determining the overall CL performance, as it depends on these vital elements. This section will provide a description of the functions and technical impacts of the CLs.

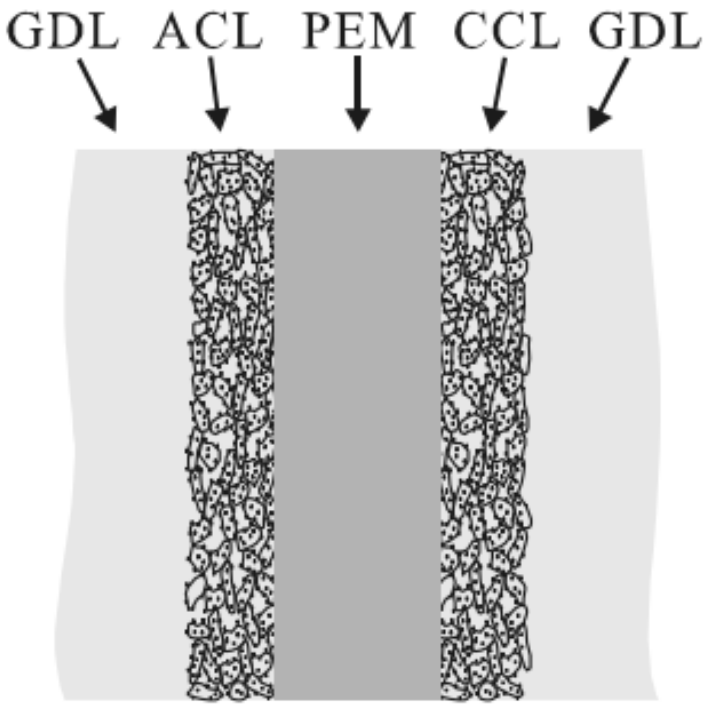


Figure 2.3: Schematic diagram of a catalyst layer structure

2.4.3 Gas Diffusion Electrodes

The GDE is the central element of PEMFCs, and it has a crucial impact on both the performance and cost of the fuel cell. The GDL and CL make up the GDE. The CL is responsible for the hydrogen oxidation reaction (HOR) at the anode and the oxygen reduction reaction (ORR) at the cathode. As a result, the CL significantly affects the performance and durability of PEMFCs.

The electrode area comprises a gas transport substrate that fulfils the functions of current collection and gas transport. GDEs are primarily distinguished by their thickness, which ranges from 100 µm to 300 µm, and their porosity. The integration of the membrane, gas-diffusion layer, and catalyst is referred to as the MEA.

2.4.4 Bipolar Plates

Bipolar plates (BPs) are integral to the functionality of PEM fuel cells, fulfilling a variety of roles. These include distributing fuel gas and air uniformly, facilitating electrical current flow between cells, dissipating heat from the active area, and sealing off gases and coolant. In PEM fuel cell stacks, BPs are significant contributors to the overall volume, weight, and cost.
Recent scholarly analysis by Mehta and Cooper [25] delved into the design and manufacturing aspects of PEM fuel cells, specifically for vehicular applications. This study also encompassed an examination of the technical characteristics of BP materials. Borup and Vanderborgh [26] previously provided an incisive summary regarding various materials used for BPs. Furthermore, in an in-depth investigation into the design of bipolar plates for PEM fuel cells, Cooper [26] outlined multiple desirable attributes for BP materials, highlighting their importance in the overall efficiency and effectiveness of the fuel cells. The BPs have the following functions to execute:

- The purpose is to disperse the fuel and oxidant throughout the cell.
- To enhance cellular water management.
- To isolate specific cells within the stack.
- To conduct electric current away from the cell.
- In order to streamline the regulation of thermal energy.

2.5 Balance of Plant (BoP)

The term Balance of Plant (BoP) consists of different components of a fuel cell system except the fuel cell module (stack). The BOP is responsible for maintaining optimal

conditions for the stack and facilitating the distribution of power according to demand. It plays a crucial role in ensuring the efficient, reliable, and safe operation of the entire system.

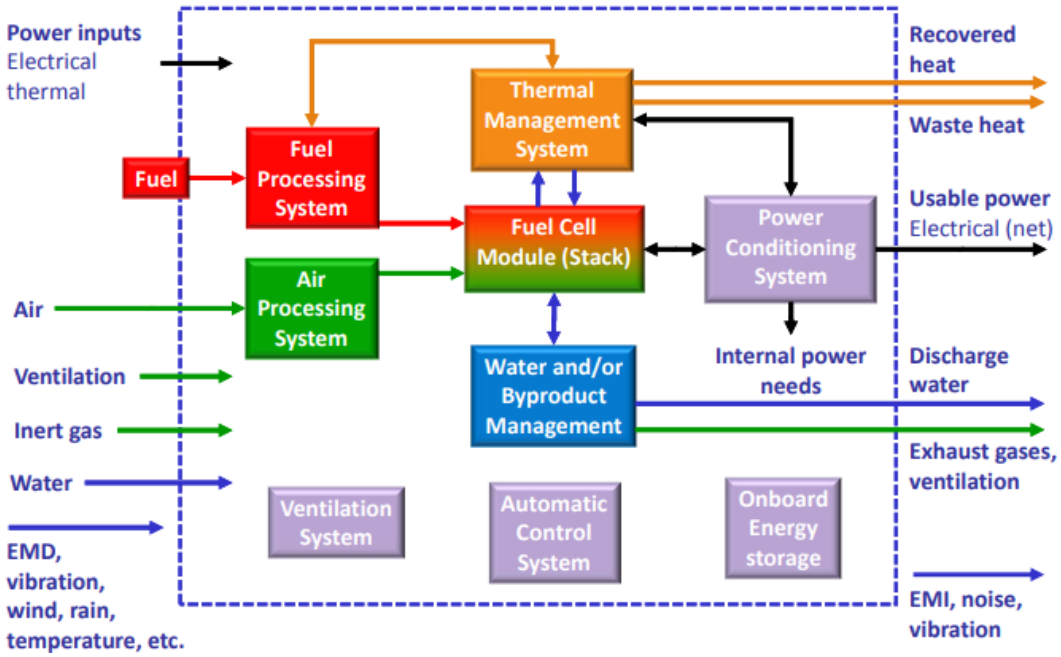


Figure 2.4: Fuel Cell System according to IEC 62282-1

2.5.1 Major Components of BoP

Fuel cell systems rely majorily on five primary sub-systems namely Fuel processing system, Air processing system, coolant/thermal management system, water management system and power conditioning system. Water management system can be incorporated together along with anode and cathode subsystems. While these components do not directly participate in the electrochemical process, they are crucial for supporting the functioning and enhancing the efficiency of the PEMFC. A simple overview of Fuel Cell System according to IEC 62282-1 is shown in fig 2.4

Anode Sub System

Fuel processing system or sometimes called as anode subsystem as shown in fig 2.6 ensures the functioning of the PEMFC as it guarantees the reliable and effective delivery of hydrogen to the fuel cell, enabling the most efficient production of power.

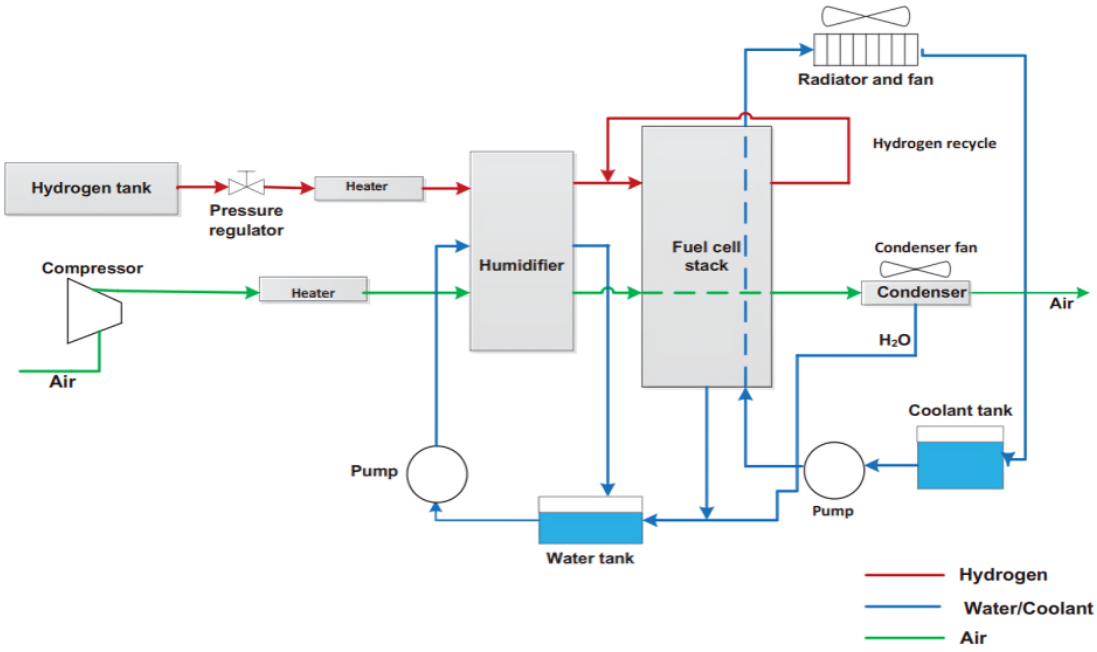


Figure 2.5: Schematic diagram of PEMFC system

The design is meticulously crafted to achieve a harmonious balance between efficiency, safety, and reliability. Each individual component must be meticulously regulated to ensure seamless coordination with the others. Various components that comes under anode subsystem are:

1. **Hydrogen Tank:** It contains the fuel (hydrogen) at high pressures in the ranges of 35 MPa to 70 MPa. Given that hydrogen is not widely available fuel there are only few common ways available to store it [4].

- compressed gas.
- as a liquid.
- as metal hybride.

2. **Pressure regulator:** It is an essential safety and control element. It decreases the high pressures of hydrogen that is flowing out of tank to a lower or controllable pressure which is required in the operation of the fuel cell stack. This guarantees that the hydrogen is transported at a uniform and secure pressure, preventing any harm to the stack.

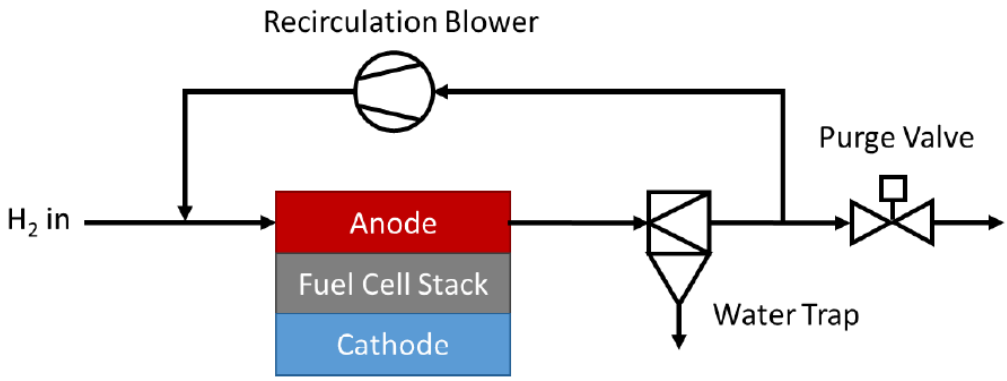


Figure 2.6: Main components of fuel processing system

3. **Recirculation pump:** Only a certain portion of hydrogen that enters the fuel cell stack is utilised in the generating the energy. This is where a recirculation pump/blower handles the work of reintroducing the unused hydrogen back into the back into the anode supply stream. This not only guarantees a maximum utilisation of the fuel but also enhances the efficiency of the system.

4. **Purge/Relief valve:** Over time, there is a possibility for the accumulation of inert gases, like nitrogen, on the anode side. This can occur due to the transfer of gases from the cathode side or the presence of these gases in the hydrogen fuel. The purge valve is employed to periodically discharge these gases from the system in order to avoid the dilution of the hydrogen fuel, which may lead to a deterioration in the performance of the fuel cell.

5. **Water Management in the Anode Subsystem:** Water management is crucial in the anode subsystem of PEMFCs to maintain proper membrane hydration and prevent anode flooding. Ensuring adequate moisture levels in the membrane is vital for preserving its ability to conduct protons, which is critical for the optimal functioning of fuel cells. Concurrently, the system must handle the water generated during the electrochemical process to avoid floods, which might impede the passage of hydrogen to the catalyst sites. The equilibrium between the reactants is crucial for ensuring a continuous supply of hydrogen and achieving the most efficient reaction rates, which directly influence the performance and longevity of the fuel cell.

Cathode Sub System

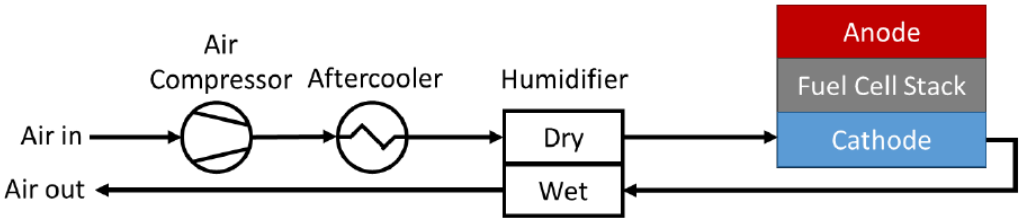


Figure 2.7: Main components of air processing system

The air processing system or cathode subsystem is a fundamental component of fuel cell systems. It facilitates the regulation and delivery of oxygen to the cathode in support of the electrochemical reactions occurring within the fuel cell. The cathode and its associated subsystem are crucial for ensuring the proper functioning of the fuel cell, particularly in managing reactant flow and pressure, as well as maintaining optimal humidity levels. Additionally, the dynamics of the air processing system include regulating the oxygen supply to prevent oxygen starvation within the fuel cell and to achieve efficient power generation [26]. compressor and humidifier are two most important components of cathode subsystem as shown in fig 2.7.

1. **Compressor:** In a PEMFC system, the compressor plays a crucial role in delivering air to the cathode and ensuring the required pressure for efficient oxygen transport within the fuel cell. It typically consumes a significant amount of power, affecting the overall system efficiency. The efficiency of the compressor is vital as it directly impacts the overall energy consumption of the fuel cell system. The compressor should operate within optimal efficiency levels to minimize energy losses and enhance the performance of the PEMFC.

2. **Humidifier:** The humidifier aids in maintaining the required level of moisture within the fuel cell, which is critical for sustaining optimal performance. By controlling the humidity of the reactant gases, the humidifier influences the proton conductivity of the membrane, which is integral to the functioning of the PEMFC. Efficient humidification ensures proper water management within the fuel cell and contributes to maximizing its performance.

3. **Water Management in the Cathode Subsystem:** The primary objective of water management in the cathode subsystem of PEMFCs is to eliminate the water generated as a byproduct of the electrochemical reaction. Effective elimination is essential to avoid cathode flooding, ensuring the uninterrupted and effective dispersion of oxygen to the catalyst sites. In addition, the management of water in the cathode aids in temperature regulation by facilitating the dissipation of heat created during operation by the elimination of surplus water. It is crucial to minimise overheating in order to avoid the deterioration of important parts and to ensure that the fuel cell operates at optimal efficiency and lasts for a long time.

Coolant/Thermal Management System

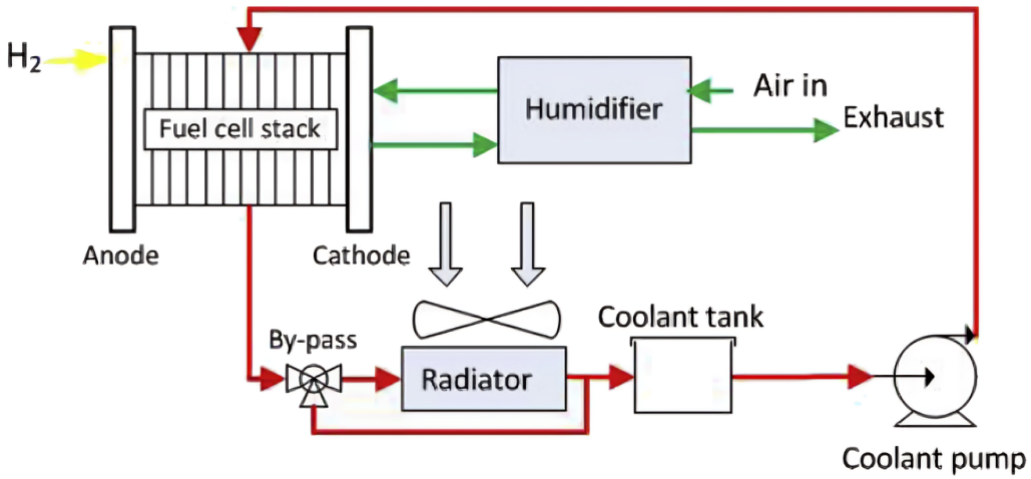


Figure 2.8: Main components of coolant/thermal management system

The thermal management system (shown in fig 2.8 [27]) within a PEMFC is responsible for regulating the temperature to enable efficient operation. This includes maintaining the proper operating temperature of around 80°C for PEM fuel cells, as well as managing the dissipation of heat generated during the electrochemical reactions. Additionally, the coolant system supports the PEMFC by actively dissipating heat, preventing temperature overshoot, and ensuring fast warm-up without consuming excessive auxiliary power.

1. **Radiator:** The radiator in the coolant subsystem of a PEMFC plays a critical role in managing the thermal dynamics within the fuel cell system. The coolant circulation pump and radiator are integral components responsible for removing heat from the fuel cell and associated components. The efficient operation of the radiator in the coolant subsystem ensures that the PEMFC operates under the required thermal conditions, enabling reliable and optimal performance of the fuel cell stack.

Power Conditioning System

Power conditioning system in PEMFC [28] fig 2.5 The primary function of the power conditioning system is to transform and optimise the electrical output generated by the fuel cell, making it suitable for utilisation by external circuits.

Fuel cells normally produce a low DC voltage, hence multiple fuel cells are commonly connected in series to provide a greater voltage. Nevertheless, it may be necessary to modify the voltage (either increase or decrease it) in order to meet the specific needs of the electrical equipment or adhere to the criteria set by the electrical grid.

Numerous applications necessitate AC power, whereas fuel cells produce DC power. The inverters inside the power conditioning system transform the DC output into AC with the required voltage and frequency.

The power conditioning system guarantees the integrity of the electricity by eliminating any electrical interference and stabilising the output to deliver a consistent and dependable power supply.

The system has mechanisms to regulate the amount of power generated, ensuring the protection of both the PEMFC and the devices it supplies power to. It guarantees that the present current and voltage remain within secure and effective operational thresholds and can also isolate the fuel cell stack in the event of a malfunction.

The power conditioning system is designed to optimise efficiency by minimising losses introduced by energy conversion processes, hence ensuring a high overall system efficiency.

2.5.2 Different aspects of BoP in PEMFC Systems

The BoP is crucial in determining the overall efficiency of PEMFC systems. The performance of the fuel cell is directly influenced by the efficiency of crucial elements, such as air compressors and heat exchangers. Effective thermal management, a crucial component of BoP, is necessary to ensure that the fuel cell operates within its optimal temperature range. This not only eliminates excessive heat generation but also guarantees the durability of the system.

Ensuring the upkeep of BoP components is essential for the uninterrupted and dependable functioning of PEMFC systems. This entails routine inspections and maintenance of diverse elements such as compressors, heat exchangers, and humidifiers. The costs associated with maintaining the BoP can be substantial, including expenses for replacement parts, labour, and the time lost during maintenance tasks.

The influence of the BoP on the efficiency and commercial feasibility of PEMFC systems is substantial. The effectiveness of BoP components has a direct impact on the overall efficiency of the system. For instance, a more effective compressor can reduce the energy needed for operation, hence improving the overall output of the system. Moreover, the expense and intricacy of BoP are significant factors in assessing the commercial feasibility of PEMFCs. Streamlining the design of BoP and minimising its expenses are crucial focal points of current investigations with the objective of enhancing the competitiveness of PEMFCs in comparison to alternative energy technologies.

One of the main difficulties in this area is the efficient and economical integration of BoP components, especially for mobility applications like cars. The future outlook for the area appears optimistic, as developments in materials and technology are anticipated to result in BoP components that are more efficient, dependable, and economical. These advancements are expected to enhance the attractiveness of PEMFC systems for a wider variety of uses.

3 PEMFCS Model Development

This chapter will concurrently achieve the objectives of verifying and validating the model provided below, as well as the interfaces responsible for constructing the model. Once the model demonstrates its ability to produce logical and precise outcomes, it may be relied upon as a dependable instrument for modelling and assessing fuel cells with diverse manufacturer's data sheet configurations, which aligns with the study objective outlined in Chapter 1. A comprehensive explanation of the interfaces responsible for building these models will be provided in subsequent chapters. The developed stack model integrates features from both chemical and electrical domains, adapted for use with electrical simulation programs to reflect the impact of operating parameters on fuel cell performance, based on the article provided by Tremblay and Dessaint (2009) [29] in their work on a generic fuel cell model for Simulink .

This model is implemented in SIMULINK (Simscape) to serve as a general-purpose model that can be adapted for more complex systems. It effectively captures the dynamic behavior of Proton Exchange Membrane Fuel Cells (PEMFCs) based on various operating parameters. This model is adapted for the use in openModelica an open-source modelling and simulating software which allows for easy integration into different modelica supported platforms (for eg: Dymola).

3.1 Model Assumptions and Limitations

- The gases, hydrogen and oxygen, that are part of the PEMFC process are considered to closely follow the rules of an ideal gas. This indicates that the gases adhere to the ideal gas law without any aberrations, hence streamlining calculations pertaining to volume, pressure, and temperature.
- The fuel cell stack is continuously supplied with pure hydrogen and ambient

air. By making this assumption, we may ignore impurities or differences in the composition of the reactants, which could otherwise affect the reaction rates, cell voltage, and overall efficiency of the fuel cell. By presupposing a consistent and untainted provision, the model may concentrate on idealised reaction kinetics and energy transformation mechanisms. Mixed gas composition may be considered in future, allowing for a more comprehensive analysis of the system's performance.

- The PEMFC stack is fitted with a cooling subsystem that can effectively maintain a consistent temperature for the stack, regardless of various operating conditions.
- The fuel cell assumes a hypothetical presence of a water management system to precisely control the humidity level within the cell. This mechanism is presumed to be efficient, ensuring the optimal moisture level in the membrane to enhance proton conductivity and prevent both excessive water accumulation and dehydration of the cell. Maintaining a consistent level of humidity is crucial for preserving the membrane's functionality, particularly when subjected to fluctuating loads.
- In the flow channels of the PEMFC, the pressure drops are so insignificant that they may be ignored. This assumption streamlines the study of fluid dynamics within the cell by eliminating the requirement to compute pressure gradients and their impact on the rates at which reactants and products flow. By disregarding these pressure drops, the model may focus on the electrochemical components of fuel cell functioning without considering intricate fluid flow patterns.
- The model assumes that the voltage reductions across the fuel cell are only caused by the reaction kinetics and the transmission of electrical charge. It is assumed that the cell functions beyond the region where mass transit is limited, which would otherwise result in substantial losses caused by the reduction of reactants at the reaction sites. By making this assumption, we may concentrate on improving the kinetics and charge transport pathways in order to enhance the performance of the cell.
- The constant cell resistance refers to the electrical resistance within the cell, which remains unchanged regardless of the operating conditions, including load, temperature, or humidity. The presence of a constant resistance in the electrical model of the fuel cell allows for a more simplified analysis. This resistance remains consistent and can be used to accurately calculate voltage drops and power production under various operational conditions.

- This model does not take into consideration the phenomenon of fuel crossover, which is the movement of gases or water through the membrane. This indicates that the membrane is very discerning, effectively preventing the blending of fuel and oxidant streams, hence avoiding any efficiency losses that may be linked to it. The absence of crossover simplifies the concerns related to mass transfer and directs the analysis towards the desired electrochemical pathways.

- The influence of temperature and humidity fluctuations on the stack resistance is disregarded. This assumption proposes that the ionic conductivity of the membrane and the contact resistance inside the cell components remain constant regardless of variations in ambient conditions or the operational state of the fuel cell.

- The model limits the capability to analyse heat generation and dissipation within the cell, as well as the following temperature gradients. Assuming that the temperature remains evenly distributed and consistent, as regulated by the cooling subsystem. Hence, this model's predictive capabilities do not encompass thermally generated stresses or variations in material properties caused by temperature fluctuations. This enables the attention to be directed towards the electrochemical and fluid dynamic behaviours, while disregarding the complications arising from heat impacts on the performance of the PEMFC system.

3.2 OpenModelica: Modelica modelling language

Modelica is a powerful object-oriented, equation-based language used for modeling complex physical systems. OpenModelica, an open-source implementation of the Modelica language, has become increasingly popular as a simulation tool due to its wide range of features and capabilities. This section provides a comprehensive overview of Modelica and OpenModelica.

Modelica language is a modeling language used to simulate complex physical systems. It is an object-oriented language that allows for the creation of reusable components and models. OpenModelica, an open-source implementation of the Modelica language, provides a comprehensive simulation environment that supports multi-domain modeling, including mechanical, electrical, thermal, and hydraulic systems. This makes it

an ideal tool for simulating complex systems that involve multiple domains. The Modelica language and OpenModelica offer a wide range of features and capabilities that make it an ideal simulation tool. For example, the language provides a high-level of abstraction, which allows for the creation of complex models with ease. Additionally, the language supports the use of libraries and predefined components, which simplifies model development and reduces modeling errors.

OpenModelica provides a user-friendly integrated development environment (IDE) that simplifies the process of model development, simulation, and analysis. The simulation environment supports parallel simulation, optimization, and sensitivity analysis, which allows for the efficient and accurate simulation of complex systems. The user interface provides easy model editing, visualization, and result analysis, which makes it an ideal tool for both novice and experienced users. The simulation workflow in OpenModelica is well-defined and easy to follow. The process begins with the creation of a model, which can be done using the Modelica language or by using the graphical user interface. Once the model is created, it can be simulated, analyzed, and optimized using the simulation environment. The results can then be visualized and analyzed using the user interface.

The equation-based modeling approach used by Modelica language and OpenModelica allows for the efficient and accurate simulation of complex physical systems. The approach enables the creation of models that are based on mathematical equations, which makes it easy to simulate systems with multiple domains. Additionally, the multi-domain modeling capability allows for comprehensive system-level analysis, which makes it an ideal tool for simulating complex systems. The use of libraries and predefined components in Modelica language and OpenModelica simplifies model development and reduces modeling errors. This makes it easier for users to create models that accurately reflect the behavior of physical systems. Additionally, the use of libraries and predefined components allows for the reuse of models, which reduces the time and effort required to create new models.

3.2.1 Important terminology

- **Package:** A package in Modelica is a collection of related classes and other packages. It provides a way to organize and structure the model components.

Packages can be used to group models, functions, and other elements together for better organization and reusability.

- **Model:** A model in Modelica represents a physical or conceptual system. It consists of components, connections, and equations that describe the behavior and interactions of the system. Models can be used to simulate and analyze the system's dynamic behavior.
- **Block:** In Modelica, a block is a type of model that represents a system or component with inputs and outputs. It can be used to encapsulate functionality and provide a modular approach to system modeling. Blocks can be connected together to form larger systems.
- **Partial model:** A partial model in Modelica is a model that defines only a subset of the components and equations required to fully describe a system. It can be used as a template or base model that can be extended or specialized by other models. Partial models allow for code reuse and provide a way to define common behavior that can be shared across multiple models.
- **Record:** A record is a data structure that contains multiple fields or attributes, each with its own name and value. It is used to group related data together and organize it in a structured manner.
- **Function:** A function is a reusable block of code that performs a specific task. It takes input parameters, performs operations on them, and returns a result. Functions can be used to encapsulate logic and make code more modular and reusable.
- **Redeclare:** The redeclare keyword in Modelica is used to modify or override the properties of a component or model that is inherited from a base class. It allows for customization and specialization of models without modifying the original definition. Redeclaration can be used to change properties such as parameter values, variable types, and equations.
- **Replaceable:** The replaceable keyword in Modelica is used to define a component or model that can be replaced with a different implementation. It allows for flexibility and modularity in system modeling by enabling the substitution of components without modifying the overall system structure. Replaceable components can be used to create reusable libraries and facilitate model customization.

3.3 Modelling Approach

This section discusses the process of modeling PEM Fuel Cell systems using OpenModelica. The process starts with setting up the OpenModelica environment, which is then integrated with existing and future models. The stack model is selected through a literature review and customization for OpenModelica. Initially, the system architecture is built by defining all the required interfaces (Stack, Anode Subsystem, Cathode Subsytem, Coolant Subsystem and Feedback Control System). The stack interface model is built, incorporating all internal components and ensuring modular design for future integration. Subsystem interfaces are identified and mapped, and the Proportional-Integral (PI) control system is implemented. The PI controller is designed and functioned, and its role is discussed in maintaining operational stability. The chapter concludes by highlighting how this modeling approach addresses current needs of PEM Fuel Cell system simulation and provides a versatile foundation for future enhancements and integration with different stack models. The use of OpenModelica, combined with insights from the MATLAB model, provides a robust platform for accurate and efficient simulation of PEM Fuel Cell systems.

3.4 Setting Up the Environment

To setup an environment in OMEdit for modeling a PEM fuel cell system involves organizing various components and blocks into a coherent structure. This ensures that the model is both modular and easily navigable. The provided fig 3.23.1 illustrate the process of creating a new Modelica class and the hierarchy of packages and components within the PEM Fuel Cell library in OMEdit.

3.4.1 Procedure for Creating a New Modelica Class in OMEdit

To create a new Modelica class in OMEdit, the process is simplified and straightforward. First, navigate to the "File" menu and select the option for creating a new Modelica class. This step initiates the creation of a new component within your model. During this process, you will be prompted to provide a name for your new class. The name chosen should be descriptive, accurately reflecting the class's role within the PEM fuel cell system.

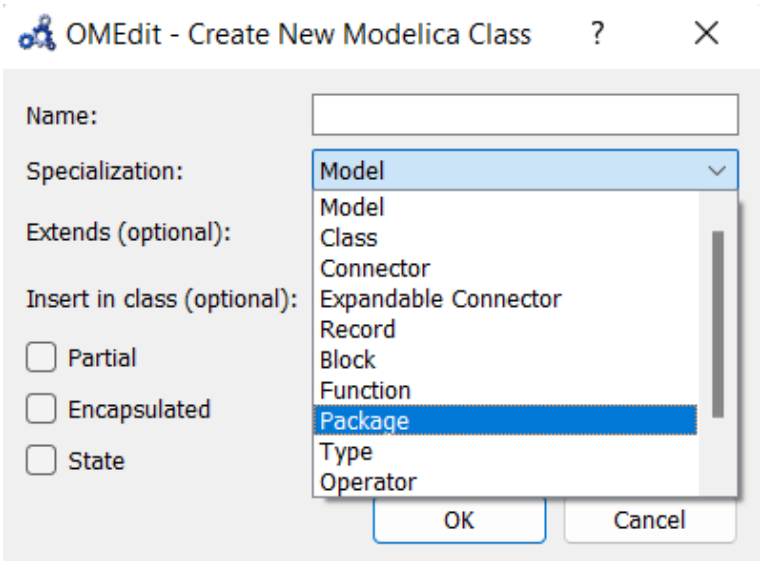


Figure 3.1: Model creation

Subsequently, choose the specific specialisation for your newly created class. The offered alternatives encompass 'Model,' 'Class,' 'Connector,' 'Record,' 'Block,' 'Function,' 'Package,' 'Type,' 'Operator,' and more choices. Each of these categories has a distinct purpose, addressing various areas of system modelling. For instance, the term 'Model' refers to the mathematical depiction of a system, 'Connector' pertains to the development of interfaces, 'Block' is used to connect inputs and outputs, and 'Package' is employed to organise different components.

If your new class needs to extend from an existing class, there is an option to specify this. Finally, after setting up these properties, simply click "OK" to create the class with the chosen specifications. This streamlined process allows for efficient and organized development within the Modelica environment.

3.4.2 Understanding the Package Hierarchy and Components

The PEM Fuel Cell library is structured to encapsulate the entire PEM fuel cell system's components and their interactions. Here's an overview of the package hierarchy and components:

– **Interfaces Package:** This contains definitions for the interfaces of the fuel cell

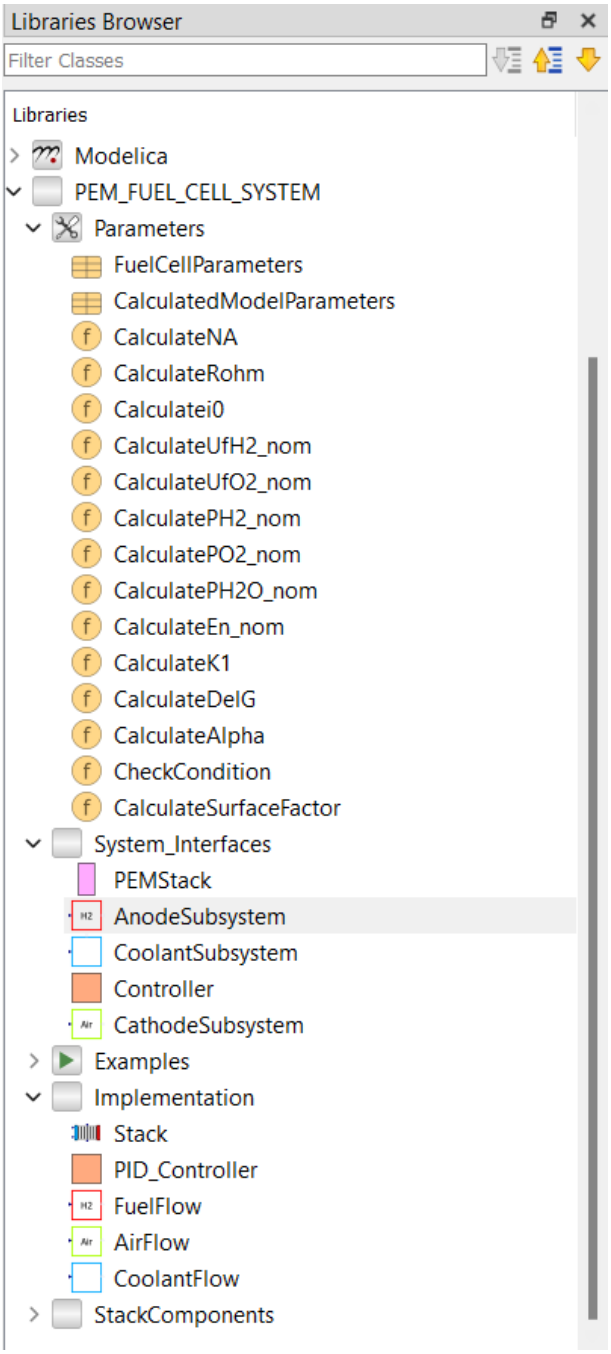


Figure 3.2: Model Library Setup

stack (FC STACK) and subsystems such as hydrogen (H2), air, and coolant. These interfaces will later be used to connect the stack to its respective subsystems, facilitating the flow of materials and information.

- **Examples Package:** This includes example models like 'SystemArchitecture' that demonstrate how the components can be assembled into a complete system.
- **Implementation Package:** Houses the actual implementation of the fuel cell stack model ('FuelCellStack') and the logic for the Proportional-Integral-Derivative (PID) controller ('PID controller').
- **Utilities Package:** Contains utility classes such as 'Parameter records,' 'Flow Parameters,' 'Constants,' and 'Calculated ModelParameters.' These are essential for defining the physical and operational parameters that the PEM fuel cell model will use.
- **Functions Package:** This includes a collection of functions like 'CalculateNA,' 'CalculateRohm,' etc. These functions are mathematical expressions that calculate specific properties or parameters based on the inputs they receive. They are crucial for defining the behavior of the PEM fuel cell system and will be invoked by the stack model during simulation.

Each package and component plays a specific role in constructing the PEM fuel cell model. For instance, the 'Interfaces' package ensures that all parts of the fuel cell, such as the anode, cathode, and coolant systems, can interact seamlessly. The 'Implementation' package is where the core functionality of the model resides, and it will directly utilize the parameters and functions defined in the 'Utilities' and 'Functions' packages to simulate the behavior of the fuel cell. With this environment setup, we lay the groundwork for a comprehensive PEM fuel cell model.

3.5 System Architecture

The fig 3.3 illustrates a modular and interconnected system architecture for a PEM fuel cell system. This architecture is specifically developed for dynamic simulation and control in OpenModelica. The architecture is designed in a way that follows an

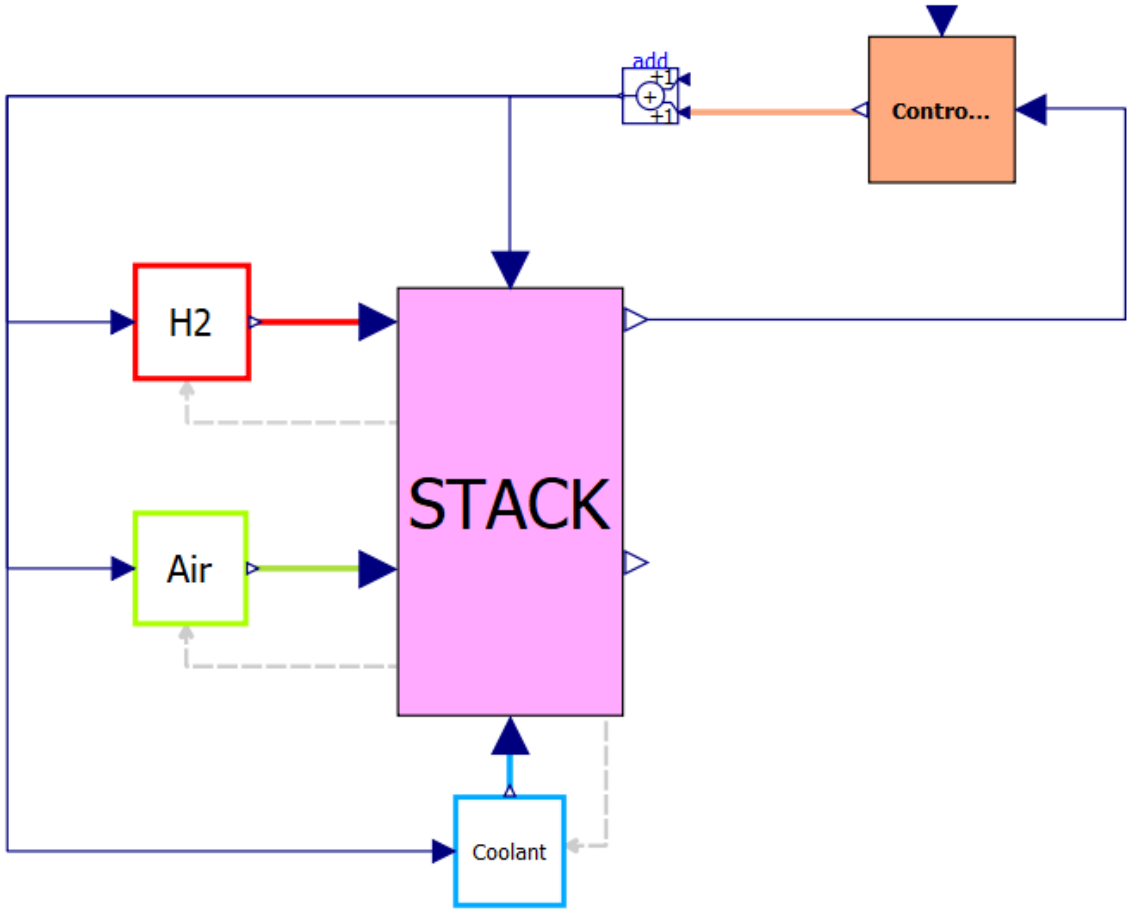


Figure 3.3: System Architecture

architecture-driven approach, highlighting the strategic interaction between different subsystem interfaces and the central control unit.

3.5.1 Overview

The following explains the interface inputs and outputs petaining to variables and parameters. The composition field introduced in the subsystems are for future improvements, which allows for more detailed characterization of the hydrogen feed and enhancing the system model capabilities.

Anode (H2):

- **Inputs:**
  - Pressure in: The incoming pressure level of the hydrogen gas.
  - Temperature: The temperature of the hydrogen feed.
  - Massflow: The mass flow rate of hydrogen entering the system.
  - Composition: The composition of the incoming hydrogen, which may include CO_2 or other gases.
  - RH: The relative humidity of the hydrogen gas.
  - Recirculation: Any hydrogen recirculated back into the anode input.
- **Outputs:**
  - Pressure out: The pressure level of hydrogen exiting the anode.
  - Temperature out: The temperature of hydrogen after reaction in the fuel cell.
  - Massflow: The mass flow rate of hydrogen exiting the system.
  - Composition: The composition of the outgoing hydrogen, potentially altered by the fuel cell reaction.
  - RH: The relative humidity of the hydrogen gas after passing through the fuel cell.

Cathode (Air):

- **Inputs:**
  - Pressure in: The pressure level of the air supplied to the cathode.
  - Temperature: The temperature of the incoming air.
  - Massflow: The mass flow rate of the air being supplied.
  - Composition: The composition of the incoming air, typically containing N_2 and O_2.
  - RH: The relative humidity of the air.
- **Outputs:**
  - Pressure out: The pressure of the air after it has passed through the cathode.

  - Temperature out: The temperature of the air after reacting in the fuel cell.
  - Massflow: The mass flow rate of air exiting the cathode.
  - Composition: The composition of the air after it has participated in the electrochemical reaction, with a reduction in oxygen content.
  - RH: The relative humidity of the air post-reaction.

PEM STACK:

- All inputs from the Anode and Cathode, along with the cooling system requirements, which include temperature, pressure, and mass flow of the coolant.
- The current demanded by the external load as an input.
- Outputs to the Anode, Cathode and coolant as a part of re-circulation system.
- The voltage or current produced by the fuel cell stack, supplied to the external load.

Coolant:

- **Inputs:**
  - Electric demand: The current demanded by the external load as an input to define the setpoint temperature for the operation of the stack.
- **Outputs:**
  - Temperature out: The calculated setpoint temperature of the coolant .

Controller:

The controller interface has two inputs and one output. The inputs are the demand from the load and the feedback signal(measured signal) which is coming from the stack as a net current.

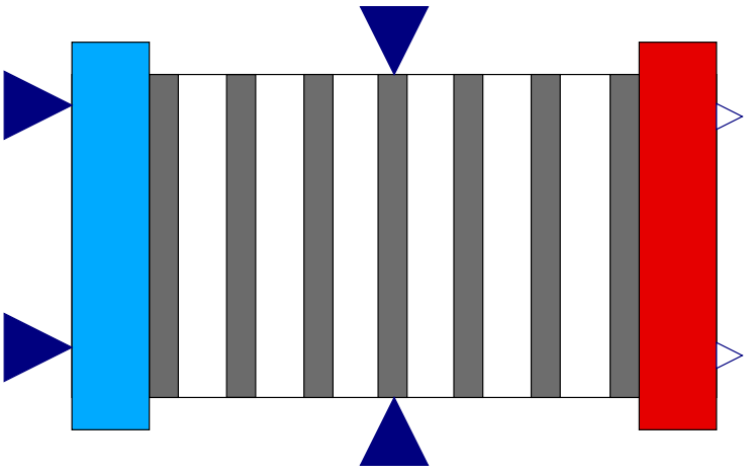


Figure 3.4: PEMFC stack interface

3.6 Fuel Cell Stack Development

A general icon view of a fuel cell stack with inputs (blue) and outputs (white) are shown in fig 3.4. This models is extended from the partial model which are defined as STACK interface in the system architecture. This model consists of several components utilising the modelica library and composed of several different models in a nested manner.

As shown in fig 3.5 the layout illustrates the internal structure of a detailed PEM fuel cell model, focusing on variable flow within the model. The Detailed Model acts as a variable hub, integrating inputs from system interfaces and producing a controlled voltage output. The inputs include multiplexed signals for temperature, hydrogen (H2), and air, representing environmental and operational conditions that affect the fuel cell's performance.

Demultiplexers receive these signals and separate them into individual data streams, used in real expression boxes on the left of the fig. Two controlled parameters, Pfuel and Pair, are set to represent operating pressures of the fuel and air supplied to the fuel cell which in turn maintains the stack pressure and which could be used to control flow rates or concentrations within the fuel cell. These parameters are set as model parameters based on the data extracted from manufacturer's data sheet.

The Detailed Model calculates the cell voltage based on the inputs it receives, which combines the features of chemical and electrical models. Adjacent to the Detailed

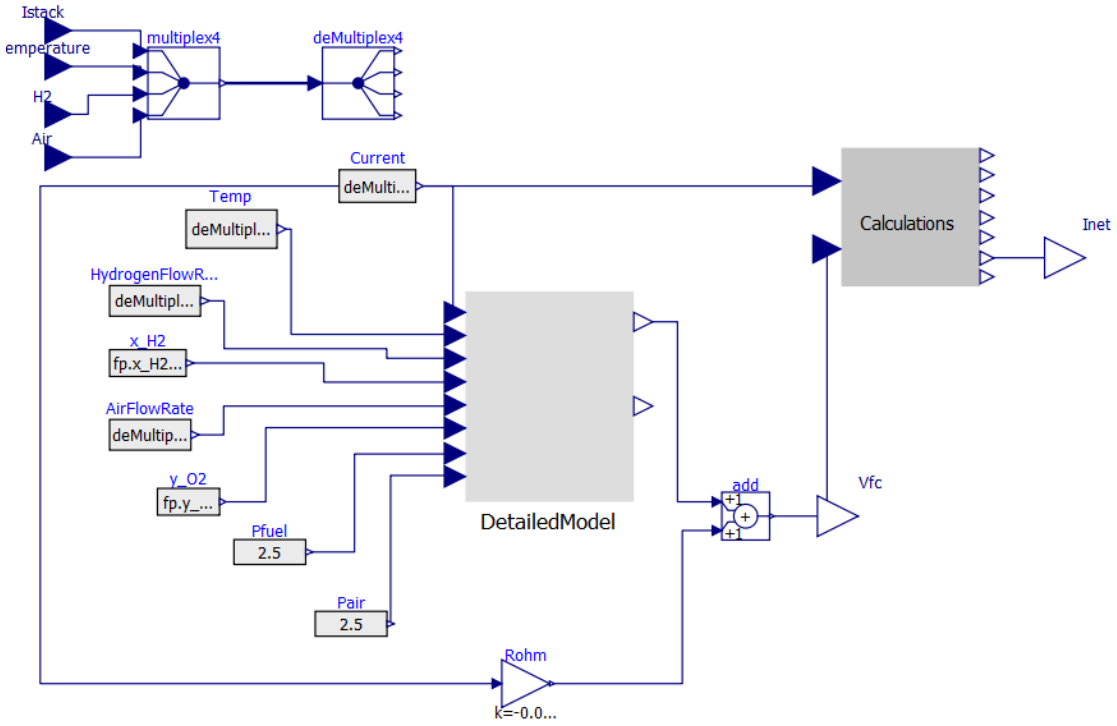


Figure 3.5: Detailed view of fuel cell stack

Model is a Calculations block, responsible for computing various power and current metrics, including Gross Power, Net Power, Gross Current, Net Current, and Gross Voltage. These calculations are crucial for understanding the fuel cell's performance and making adjustments to maintain effective control over the power generation.

The overall voltage generated by the fuel cell (V_{fc}) is calculated using the formula below:

$$V_{fc} = E - R_{ohm} i_{fc} \tag{3.1}$$

where:
V_{fc} = fuel cell voltage (V)
R_{ohm} = internal resistance(Ω)
E = controlled voltage source (V)

The output from the detailed model is a gross fuel cell voltage (V_{fc}), which directly influences the net current (I_{net}) that the fuel cell system can supply to an external

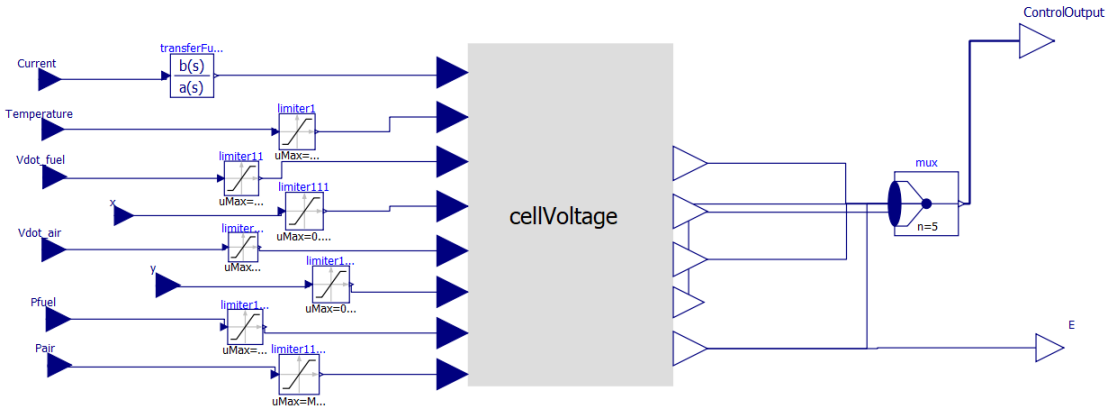


Figure 3.6: Detailed Model

load. The overall architecture of this Detailed Model is designed with an emphasis on modularity and control, taking extended inputs from interfaces corresponding to the physical conditions and components of the fuel cell system.

3.7 Detailed Model

The detailed model (see fig 3.6) model consists of several components, the cell voltage model including the transfer function, which represents the delay associated with activation losses in the fuel cell, and limiters, which act as saturation blocks to ensure the signals do not exceed specified maximum or minimum values.

The model's inputs include current, temperature, volumetric flow rate of fuel and oxidant, partial pressure of fuel and oxidant, and cell voltage. The cell voltage block calculates the voltage of the fuel cell based on these inputs.

The control output is a collective output that emerges from the mux block, which combines multiple outputs into a single vector. The combined outputs include Tafel Slope, Nernst Voltage, Exchange Current, and Open Circuit Voltage. The final output signal, labeled 'E', represents the controlled voltage source, used to represent the electrical output of the fuel cell.

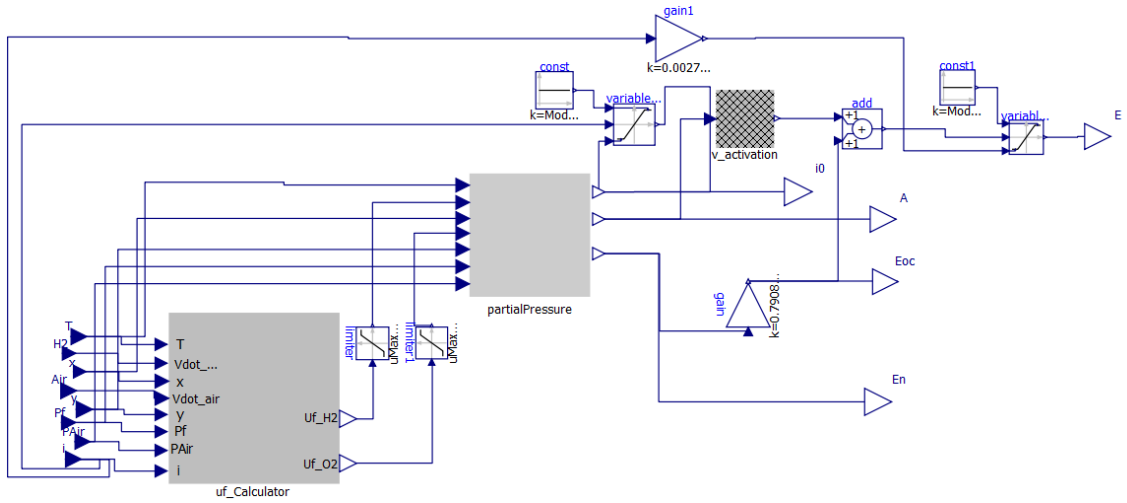


Figure 3.7: Cell Voltage

3.8 Cell Voltage

The schematic (fig 3.7) provides a detailed view of the cell voltage model for a PEM fuel cell, focusing on the calculation of cell voltage while considering utilization factors of reactant gases, partial pressures within the cell, and activation losses. The main components include the $Uf_{calculator}$, which calculates utilization factors (Uf_{H2} for hydrogen and Uf_{O2} for oxygen), the partial pressure calculator, which calculates partial pressures of reactant gases, and the $V_{activation}$ block, which calculates activation losses.

The outputs from these blocks contribute to the overall voltage calculation, while additional variables like E_{oc} (open-circuit voltage) and E_n (Nernst potential) are integrated using a summation block (add). The ControlOutput signal combines these calculations to regulate the fuel cell's operating conditions, aiming to maintain desired performance in the presence of varying operational factors.

The final output, E, represents the controlled voltage of the fuel cell, adjusted to account for efficiency and losses within the system. The integration of these components ensures accurate determination of the fuel cell's performance and efficiency.

The generic equation used for calculating the controlled voltage source (E) is given by eq 3.2:

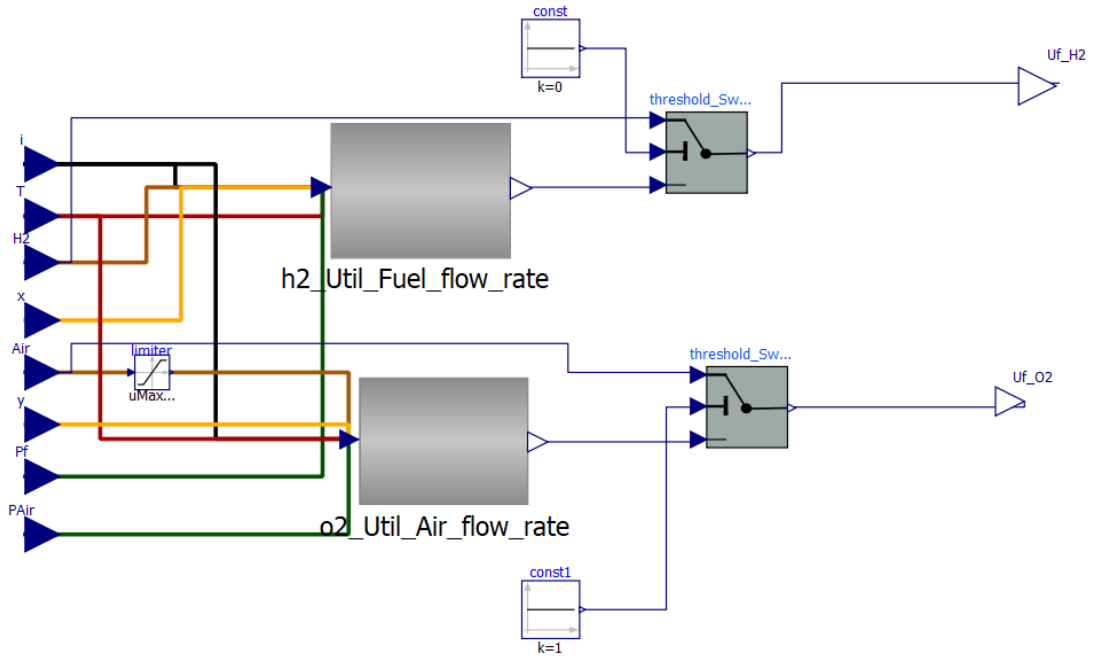


Figure 3.8: Utilization factors

$$E = E_{oc} - NA \log\left(\frac{i_{fc}}{i_o}\right) \frac{1}{s\frac{T_d}{3} + 1} \tag{3.2}$$

where:
E_{oc} = Open Circuit Voltage (V)
N = Number of cells
A = Tafel slope (V)
i_{fc} = fuel cell current (A)
i_o = exchange current (A)
T_d = the response time(sec)

3.8.1 Calculating Utilization factors

The utilization factor is defined as the fraction of the fuel/air consumed by the electrochemical reaction. It provides insight into how effectively the reactants are utilized in producing electrical energy within the fuel cell.

The fig 3.8 depicts a PEM fuel cell model, focusing on the utilization factor calculation for hydrogen and oxygen. The model calculates utilization factors (UF_H2 and

UF_O2) to determine fuel efficiency in the fuel cell. The h2_Util_Fuel_flow_rate Block uses inputs like current, temperature, hydrogen flow rate, and partial pressure of hydrogen to calculate the hydrogen utilization factor (UF_H2).

A limiter is applied to the hydrogen flow rate input to ensure it stays within operational limits. A threshold switch, can be used to activate or deactivate the flow rate calculation based on specific conditions or thresholds. The o2_Util_Air_flow_rate Block uses inputs like current, temperature, air flow rate, and partial pressure of oxygen to calculate the oxygen utilization factor (UF_O2). A limiter is also applied to the air flow rate input to maintain a specific range for the reaction. These factors are input to partial pressure block for calculating the partial pressure of the gases. The equations 3.3 3.4 define the factors based on the input to the model.

$$Uf_{H_2} = \frac{60000NRTi_{fc}}{zFP_{fuel}V_{fuel}x\%} \tag{3.3}$$

$$Uf_{O_2} = \frac{60000NRTi_{fc}}{2zFP_{air}V_{air}y\%} \tag{3.4}$$

where:
P_{fuel} = absolute supply pressure of fuel (atm)
P_{air} = absolute supply pressure of air (atm)
V_{fuel} = fuel flow rate (l/min)
V_{air} = air flow rate (l/min)
x = percentage of hydrogen in the fuel (%)
y = percentage of oxygen in the oxidant (%)

3.8.2 Partial Pressures

The fig 3.9 depicts a PEM fuel cell simulation model that focuses on the calculation of partial pressures and their use in determining the Nernst voltage, as well as other parameters critical to the fuel cell's operation. The blocks used in the model include partial pressure calculation blocks (P_{H2}, P_{O2}, P_{H2O}), limiters, threshold switch, and a multiplexer (multiplex4).

Calculation blocks (io_calc, cr, A) are used to calculate exchange current density

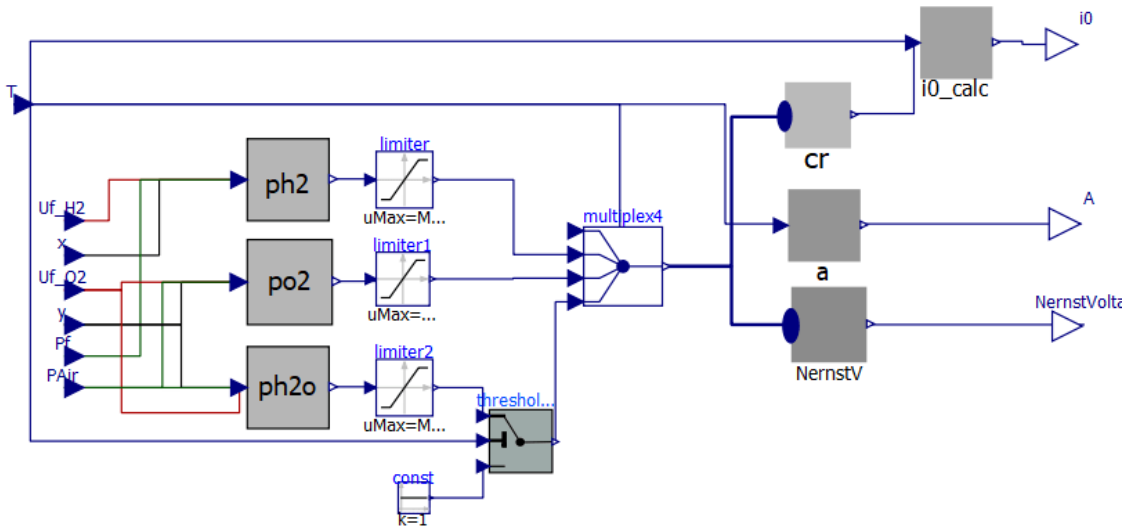


Figure 3.9: Partial Pressures

(io), a crucial parameter in determining activation losses in the fuel cell. The blocks represent constants or calculations related cr and the etafel slope (A), both of which are vital for understanding the kinetics of fuel cell reactions.

NernstV, the output labeled NernstVoltage, indicates the calculation of the theoretical maximum voltage the fuel cell can produce under standard conditions. The overall model uses the calculated partial pressures of the gases, along with operational parameters like utilization factors and pressures, to compute essential electrochemical variables. The outputs io_calc and NernstV are critical for modeling the voltage and power outputs of the fuel cell under various operating conditions. These outputs likely feed into a larger model that simulates the full operation of the fuel cell, taking into account both thermodynamic and kinetic factors to predict its performance.

The generic equation used for calculating the above parameters are:

$$P_{H2} = (1 - Uf_{H2})x\%P_{fuel} \tag{3.5}$$

$$P_{O2} = (1 - Uf_{H2})y\%P_{air} \tag{3.6}$$

$$P_{H2O} = (w + 2y\%Uf_{O2})P_{air} \tag{3.7}$$

and

$$E_n = 1.229 + (T - 298)\frac{-44.43}{zF} + \frac{RT}{zF}\log(P_{H2}\sqrt{P_{O2}}) \tag{3.8}$$

where:
P_{H2O} = partial pressure of water vapor (atm)
w = percentage of water vapor in the oxidant (%)

$$E_{oc} = K_c E_n \tag{3.9}$$

$$i_o = \frac{zFk(P_{H2} + P_{O2})}{Rh} exp\left(\frac{-\Delta G}{RT}\right) \tag{3.10}$$

where:
R = 8.3145 J/(mol K)
F = 96485 A s/mol
z = number of moving electrons (z = 2)
E_n = Nernst voltage (V)
α = charge transfer coefficient
P_{H2} = partial pressure of hydrogen inside the stack (atm)
P_{O2} = partial pressure of oxygen inside the stack (atm)
k = Boltzmann's constant (1.38×10-23 J/K)
h = Planck's constant (6.626×10-34 J s)
ΔG = activation energy barrier (J)
T = temperature of operation (K)
K_c = voltage constant at nominal condition of operation

3.9 Balance of Plant

The fig 3.10 illustrates a PEM fuel cell system, focusing on subsystem control for the anode, cathode, and coolant circuits. While the focus is primarily on these subsystems, it's essential to consider the role of the Balance of Plant (BoP) components in the overall operation of the system.

The BoP encompasses various components responsible for supporting the operation of the fuel cell stack, including but not limited to the compressor, pumps, fans, and

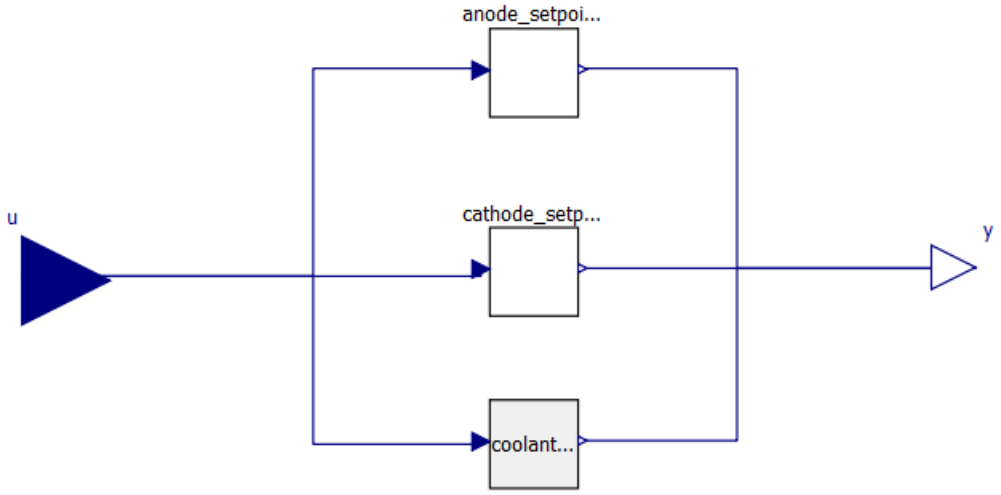


Figure 3.10: Gases flow rate calculator

thermal management systems. Among these, the compressor plays a crucial role in supplying pressurized air to the cathode side of the fuel cell.

The power consumed by the compressor which is the major power consumption part of BoP compared to the other components is calculated as a product of current consumption I_{BoP} and stack voltage V_{fc} expressed by the following equations 3.11, 3.12 & 3.13. Here the power consumed by anode and coolant subsystems are taken collectively as 10%-15% of the power consumed by the cathode subsystem.

$$W_{cathode} = \dot{m}_{air} * (c_p * \frac{T_a}{\eta_{compressor}}) * (\frac{P_2}{P_1})^{\frac{\gamma-1}{\gamma}} - 1 \tag{3.11}$$

$$W_{BoP} = W_{cathode} + W_{anode} + W_{coolant} \tag{3.12}$$

$$I_{BoP} = \frac{W_{BoP}}{V_{fc}} \tag{3.13}$$

The net current I_{net} (equation 3.14) is the effective electrical current utilized by the electrochemical reaction within the fuel cell stack, accounting for the power consumed by the BoP. It is calculated as the difference between gross current I_{stack} and BoP current I_{BoP} and is expressed as follows:

$$I_{net} = I_{stack} - I_{BoP} \tag{3.14}$$

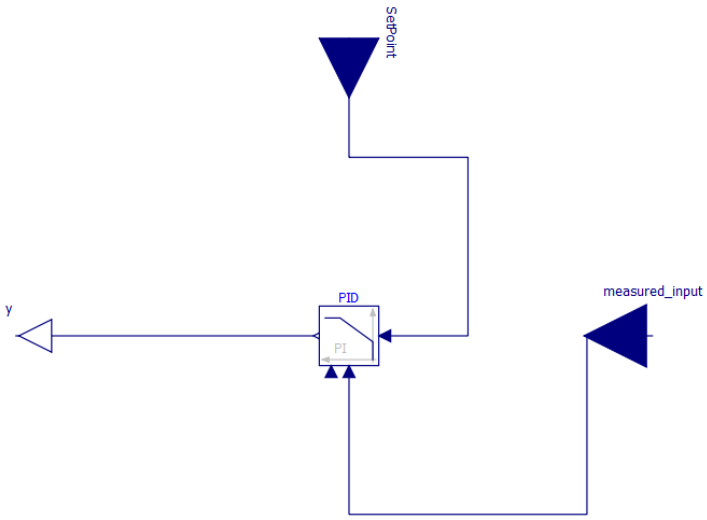


Figure 3.11: Controller

The input signal (u) represents the control input or demand signal, related to the current demand of the fuel cell system. Subsystems (anode_setpoint, cathode_setpoint, coolant_setpoint) calculate the mass flow rate of hydrogen (H_2), air (or oxygen), and fluid temperature (coolant_setpoint) to meet the current demand. These are individually calculated in their respective subsystems as discussed in the system architecture .

The subsystems receive a individual input signal and independently calculate necessary parameters to meet the demand, ensuring efficient operation by adjusting flow rates of hydrogen and air and managing coolant temperature to meet varying power requirements. Each subsystem's calculations are critical for the proper functioning of the fuel cell stack, as they directly affect the electrochemical process and overall efficiency and power output of the fuel cell system.

3.10 Feedback Control

The diagram illustrates a Proportional-Integral (PI) control loop, a crucial component in automated processes like PEM fuel cell systems. It consists of a setpoint (u_s) representing the desired value, measured input (u_m), and a controller (PID and PI)

that processes the difference between the setpoint and the measured input. The PID controller adjusts the system's output based on the error signal, integral over time effectively predicting future errors and compensating for them.

The control output (y) is the commanded output from the controller that adjusts the system's behavior, such as modulating the flow of reactant gases or adjusting the cooling system to maintain optimal operating conditions. The feedback loop is the path that the measured input takes to be fed back into the controller, crucial for dynamic systems where conditions change over time and continuous adjustment is necessary. The controller parameters are fine tune based on the system response.

Feedback control is essential in systems where precision and stability are critical. In a PEM fuel cell, maintaining the right conditions for the electrochemical reaction is vital for efficiency and longevity. The feedback control system allows for the adjustment of parameters like temperature, pressure, and flow rates within narrow ranges.

A PI controller in a PEM fuel cell system ensures the cell operates within its optimal parameters, reacting to disturbances and minimizing the error between actual operating conditions and the desired setpoints, optimizing performance, system safety, and reliability.

4 Results and Discussion

This chapter provides a thorough assessment of the PEMFC model, analysing its parameters and how accurately it represents real-world performance. The model undergoes testing against established data sheet curves and is exposed to different scenarios in order to assess its practical suitability. The accuracy of the model is assessed through a meticulous validation process, which involves comparing its outputs with a standard data sheet curve. Simulations are performed using several load profiles, such as step, ramp, trapezoidal, and conditions obtained from experimental data, in order to assess the model's resilience and ability to adapt to dynamic changes.

The polarisation curves of the model are analysed by varying the surface areas and considering the presence or absence of Balance of Plant components. The influence of PI control on the Pol curve is also examined, offering insights into the efficacy of the feedback system in preserving operational efficiency. The validation procedure is expanded by examining the impact of mass flows, subsystem pressures, and temperature fluctuations under various operating situations. Section 4.5 delves into the dynamics of the fuel cell, offering a more profound understanding of the system's temporal features. The chapter summarises important discoveries and identifies inconsistencies or mistakes, emphasising the model's advantages and limits, establishing a basis for future enhancements and research paths. The results seek to bridge the gap between theoretical modelling and real performance, providing scope for high level integration and modularity which makes the PEMFC model a dependable instrument for researchers and industry professionals.

4.1 Discussion of the developed model

The preceding chapters presented the mathematics and physical principles employed in the fuel cell model. This section elucidates the interconnection between them and

a method of computation by which the model determines the cell voltage. This section also provides an overview of the model setup and data extraction and paramters approximation.

The developed model for a PEM fuel cell system simulates the electrochemical process by taking into account the demand current (load) to determine mass flow rates of fuel and air through the anode and cathode subsystems, respectively. Variations in parameters like pressure, temperature, and composition are considered, affecting key factors such as the Tafel slope (A), exchange current density (i_o), and open-circuit voltage (E_{oc}). These factors are essential for calculating the partial pressures and Nernst voltage, which in turn influence the activation losses and overall cell voltage. The model incorporates a transfer function to account for the voltage response delay to sudden changes in stack current, considering ohmic losses with a constant cell resistance. A part of gross current generated allows for the deduction of power consumed by balance of plant subsystems, which makes the net current being less than the demand current. A PI controller is employed to adjust the mass flow rates dynamically, ensuring that the net current aligns with the demand current, demonstrating the model's capability to simulate real-world operational conditions of a PEM fuel cell system accurately.

The diagram in Figure 4.1 explains the whole work flow of the implemented model. The computation is done in a single control loop. The loop iterates until the net current meets the demand input and computes the cell voltage at each iteration by adjusting the flow rates but keeping the demand input to the stack constant until the net current meets the demand. Whereas, the demand current input accumulates over time based on the controlled output from the PI controller.

4.1.1 Data extraction and approximation of model parameters

In general, fuel cell manufacturers supply detailed specifications of their stacks, which encompass the polarisation curve, rated and peak power, cell count, efficiency, temperature, inlet pressures, and other relevant information. The data is utilised to derive the parameters of the models. Since the model developed is a generic model it facilitates several different specifications and give its modularity the satck can be easily adjusted for different sizes (surface area), voltage (in V) and power ratings (in kW).

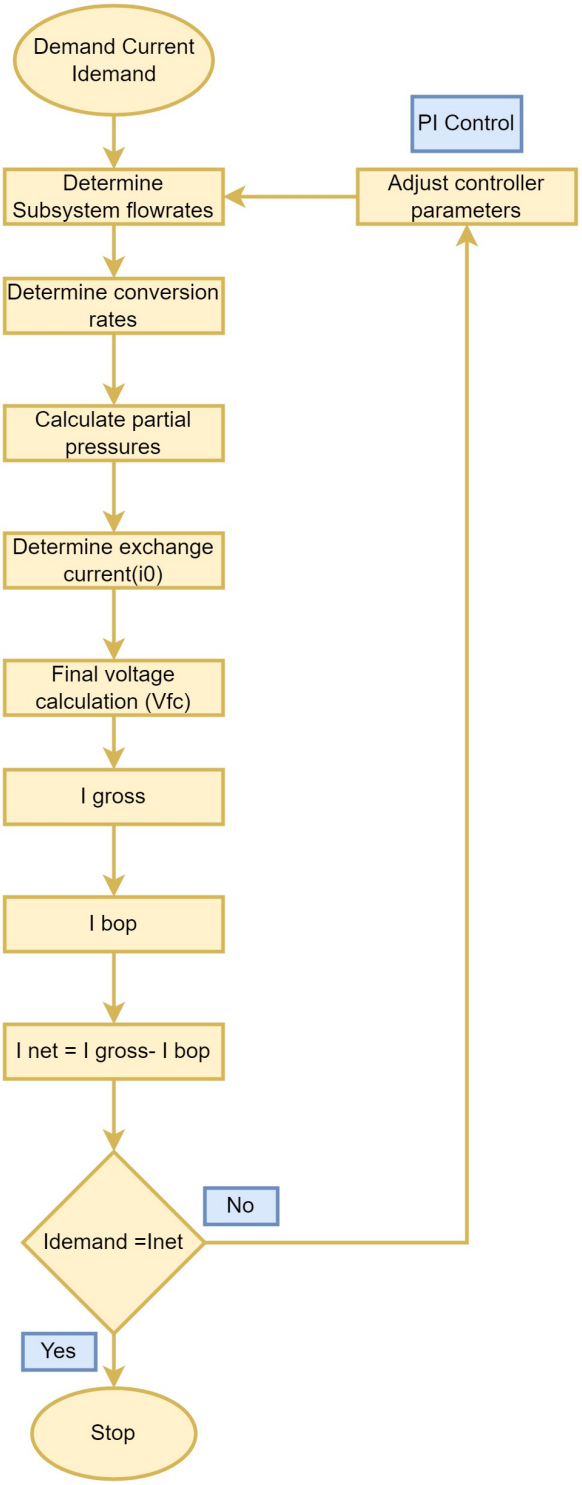


Figure 4.1: Workflow of the model

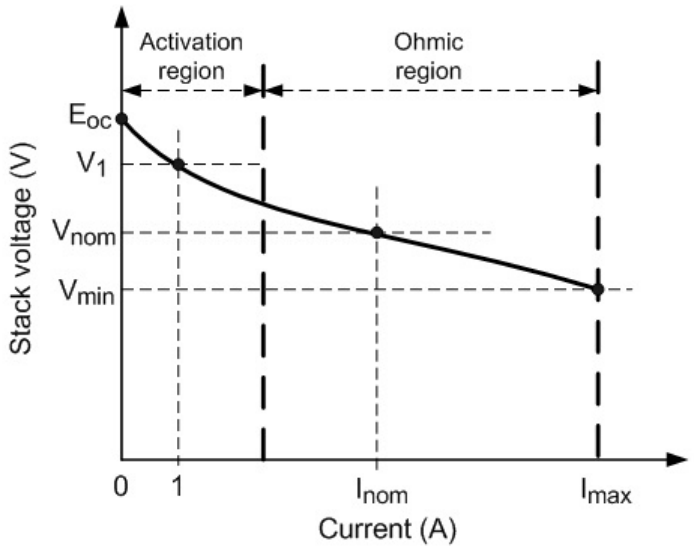


Figure 4.2: Typical polarization curve

Table 4.1 shows the essential parameters required for the model setup. These data help in determing E_{oc}, i_0, NA, R_{ohm}. The Polarization curve provided from the manufacturer helps in extracting the nominal points of operation as shown in fig 4.2 [29]. The current and voltage at nominal operating points are denoted as I_{nom}, V_{nom}. The current and voltage extreme operating points are denoted as I_{max}, V_{min}. Voltage at 0A and 1A denoted as E_{oc}, V_1.

4.2 Validation of Model with a typical data sheet curve

The model is validated for against the experimental data from the department of PEMFC and simulation is carried out to find out the accuracy. The parameters provided in table 4.1 are taken to setup the model.

To accommodate different surface areas or numbers of cells, parameters must be appropriately scaled. The factor $S2/S1$ in Table 4.1 represents the ratio of surface areas S2 and S1. This factor is applied to relevant parameters to scale them accordingly for different surface areas.

The polarization curves obtained in steady state are overlaid on the datasheet curve, as

Model Operating Parameters	
Number of cells N	300
Anode Stoichiometry λ_{anode}	1.5
Cathode Stoichiometry $\lambda_{cathode}$	2.0
Stack operating temperature T_{op}	80°C or 353.15K
Max. Stack current I_{max}	140A
Min. Stack voltage V_{min}	0.508V
Nominal stack voltage V_{nom}	0.649V
Nominal stack current I_{nom}	90A
Factor of utilization: O_2	0.5
Factor of utilization: H_2	0.6666667
Standard temperature T_{std}	273.15K
Standard pressure P_{std}	101325Pa
voltage at 1A V_1	0.932V
Open circuit voltage E_{oc}	0.969V
Nominal fuel pressure P_{fuel}	2.5atm
Nominal Air pressure P_{air}	2.5atm
Reference surface area S_1	$73.6cm^2$
Actual surface area S_2	$400cm^2$
Surface area factor S	S_2/S_1
Model Flow Parameters	
Percentage of hydrogen in the fuel x_{H2}	100%
Percentage of oxygen in the oxidant y_{O2}	21%

Table 4.1: Necessary parameters from manufacturer's data sheet

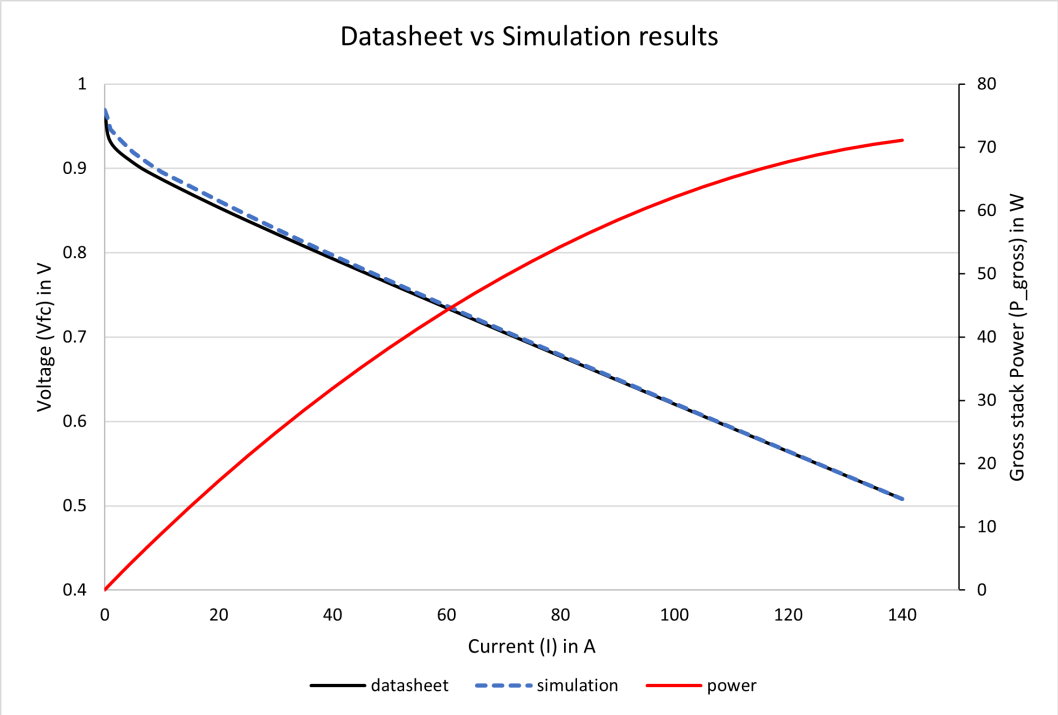


Figure 4.3: Simulation and datasheet results

depicted in Figure 4.3. The operating conditions under which the curve is obtained by taking the parameters as give in table 4.1. The accuracy of polarization curve depends on the precision of the data provided and the operating conditions under which they are obtained. An important thing to note that is the polarization curve 4.3 obtained is based on a single cell with a reference surface area S_1 . This curve provides a baseline for subsequent scaling to larger cell surfaces (covered in subsequent sections). By applying a surface factor and a cell factor, we can extrapolate the data to simulate the behavior of larger fuel cell stacks, such as those used in vehicle applications, including trucks. This scaling process allows us to gain valuable insights into the performance and efficiency of fuel cells at a scale more representative of practical applications.

The dashed line represents the simulated curve, while the solid line is the actual curve as provided in the datasheet. It is noted that the simulated curve precisely corresponds to the real curve in the ohmic zone. An observed distinction arises in the activation area as a result of the non-linear nature of the activation voltage. To obtain a more accurate value of i_0 and, additional data points are required at low current levels. Identical outcomes can be achieved with any variety of fuel cells, as they all exhibit

comparable polarization curves. The accuracy of the model is contingent upon the precision of the data provided by the user. Comprehending the operational zones of the polarization curve is crucial as they define the performance characteristics and efficiency of fuel cells under different settings. Through the analysis of the different sections of the curve, including the activation losses at low currents, ohmic losses in the intermediate range, and concentration losses at high currents, one can obtain a deeper understanding of the mechanisms that control the behavior of fuel cells.

Understanding the mechanisms behind voltage decreases at greater currents, namely concentration losses, can inform the creation of effective ways to reduce these losses. This may involve enhancing gas diffusion layers or optimizing flow channels. Similarly, comprehending activation losses can drive progress in catalyst development, with the goal of creating materials that lower the energy barrier for electrochemical reactions. Hence, the operational areas of the polarization curve not only offer a momentary assessment of a fuel cell's efficiency but also act as a guide for focused enhancements and advancements in fuel cell technology. This understanding is essential for expanding the limits of fuel cell applications, ranging from portable electronics to transportation and beyond, therefore serving as a fundamental element in the progress of sustainable energy technology.

4.3 Different basic scenarios studied

An essential aspect of comprehensively understanding the performance of a fuel cell system involves studying various fundamental scenarios, including different types of loads (such as step, ramp, trapezoidal etc). Additionally, it is crucial to examine polarization curves under different surface areas, both with and without the Balance of Plant (BOP) components. This inquiry is essential for determining the fuel cell's performance under conditions that replicate both idealized and real-world operational scenarios. Through the analysis of the system's response to many inputs, researchers can discover crucial information regarding its effectiveness, longevity, and dynamic behavior. In addition, the incorporation of PI control in these situations enables the assessment of control tactics targeted at enhancing efficiency and guaranteeing stability in the face of varying demands.

In the following sections, we will conduct thorough analysis to clarify how physical characteristics and control tactics directly affect the operational efficiency and durability of fuel cell systems. This investigation not only illuminates the fundamental electrochemical processes that support fuel cell operations, but also provides insights for the development and improvement of systems to achieve better performance. The upcoming sections analyze the system's behavior in various settings, offering a comprehensive grasp of the obstacles and possibilities in fuel cell technology. This analysis will help direct future advancements and applications.

4.3.1 Different loads (Step,Ramp,Experimental data)

Step load:

The step load analysis depicted in Figure 4.8 shows the PEM fuel cell's capacity to promptly react to abrupt variations in power requirements, a vital characteristic for practical applications. The prompt decrease in voltage and simultaneous increase in current following the application of a step load (as seen in graphs 4.4a and 4.4b) exemplify the system's rapid response, which is a favorable attribute for applications that demand both reliability and responsiveness, such as electric vehicles or emergency power systems. The graph 4.4c also illustrates a rise in the use of hydrogen and oxygen, implying that the fuel cell system effectively adjusts its chemical reactions to meet the growing energy demand. Ensuring the fuel cell's ability to retain performance under different operational situations is of paramount importance. It is important to clarify that the depicted step load analysis reflects an increase in power demand driven by an increase in current demand. When this step change in current (I_{stack}) is introduced, the variation in the output voltage (V_{fc}) and utilization factors (U_f) closely follow the step change in current.

Step load tests, as shown in the figures, are crucial for evaluating the temporary response and durability of fuel cells. These simulations replicate real-world situations characterized by frequent and sudden changes in power distribution. As a result, they yield crucial data for enhancing the design of fuel cells, particularly the Balance of Plant (BOP) components that utilize a portion of the generated power, as depicted in graph (4.4d).

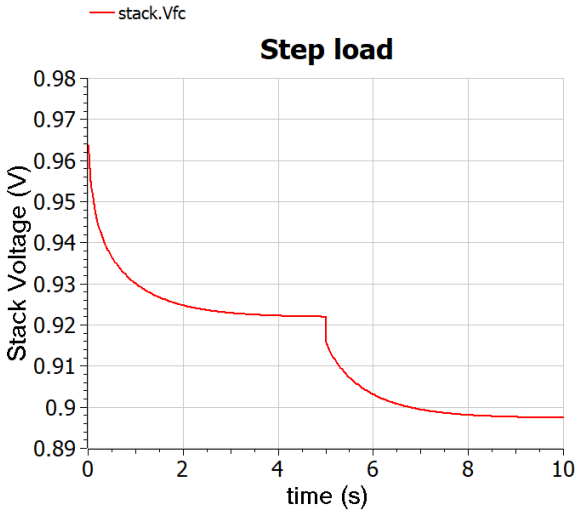


Figure 4.4: Caption 1

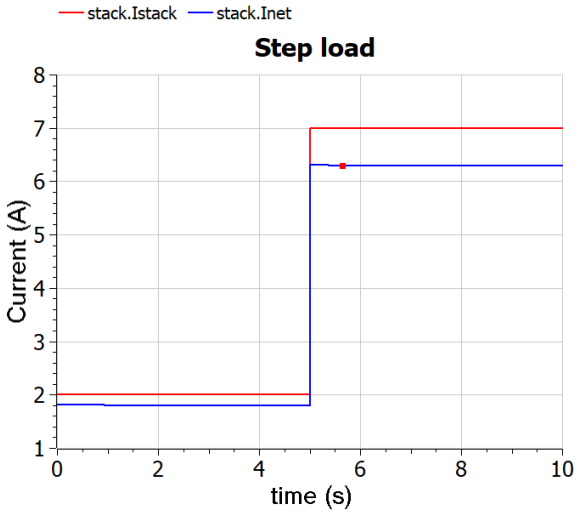


Figure 4.5: Caption 2

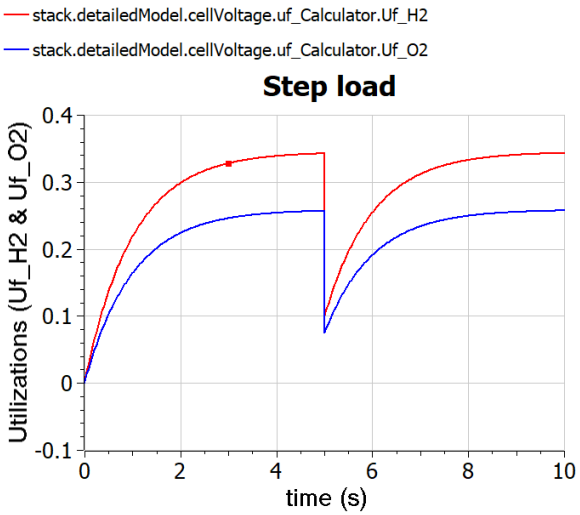


Figure 4.6: Caption 3

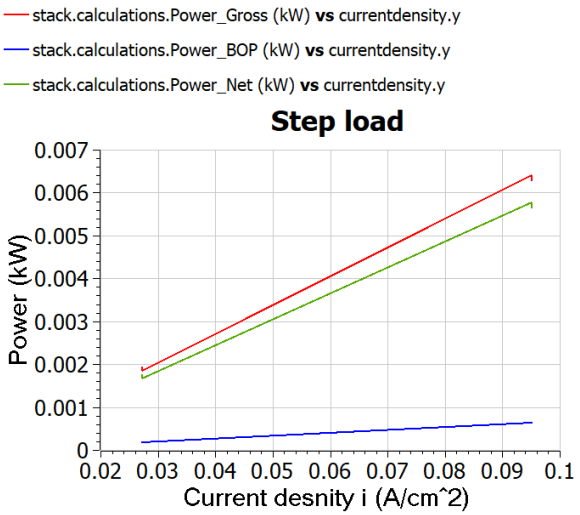


Figure 4.7: Caption 4

Figure 4.8: Step load analysis

The adaptation time T_d, representing the time taken for the voltage to stabilize after a step change in load, is a key parameter indicating the fuel cell's transient response characteristics. This phenomenon is represented in equation 3.2 by delaying the activation losses with a first order transfer function $\left(\frac{1}{sT_d/3+1}\right)$ It's essential to analyze this parameter to understand how quickly the system can adjust to changes in power demand.

Ramp load:

Figure 4.13 illustrates the analysis of ramp load for a PEM fuel cell, which is characterized by a progressive and continuous increase in power demand. The voltage response exhibits a consistent decrease as the current density increases, indicating the cell's reliable performance under higher load.

Comparison between step load and ramp load responses: A comparative analysis between step load and ramp load responses can provide valuable insights into the fuel cell's dynamic behavior under different load profiles. This comparison helps in understanding how the system adapts to varying load conditions and aids in optimizing system design and control strategies. It's worth noting that in step load tests, the adaptation time is more pronounced as the load change is abrupt, allowing for a clear evaluation of transient response dynamics. In contrast, ramp load tests may dilute the adaptation time due to the gradual increase in load, making it important to carefully analyze both scenarios for a comprehensive understanding of system behavior.

4.3.2 Polarization curve with surface area 1 and no BoP

This case explores the fundamental electrochemical performance of the fuel cell stack without the influence of BoP. The figure 4.18 provided shows various plots related to the performance of a PEM fuel cell stack under an experimental load, and how they react with different changes in the load without the Balance of Plant (BoP) components, at a given reference surface area ($S_1 = 73.6cm^2$), number of cells (N = 1), and operating temperature (T = 80°C). The absence of BoP assumes a constant mass flow through out the simulation.

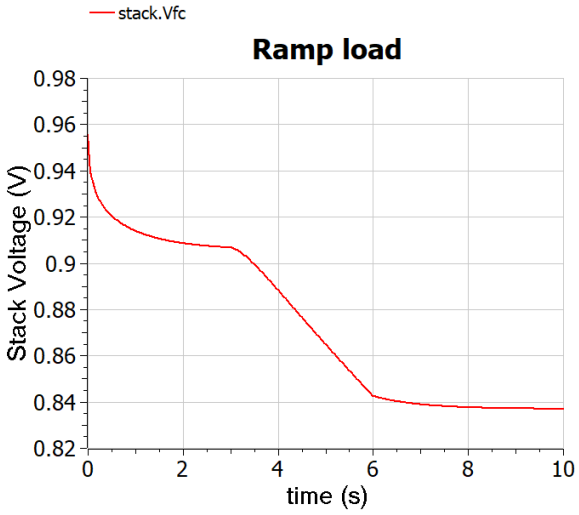


Figure 4.9: Caption for VT

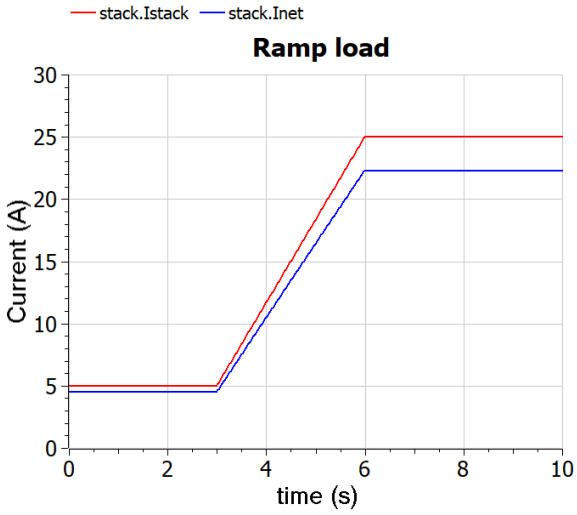


Figure 4.10: Caption for IT

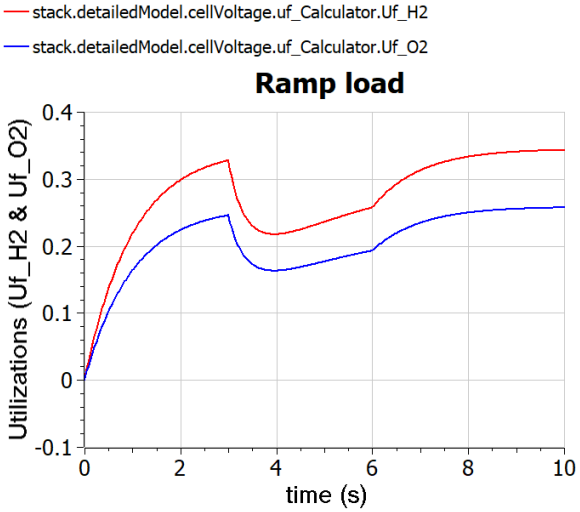


Figure 4.11: Caption for UfT

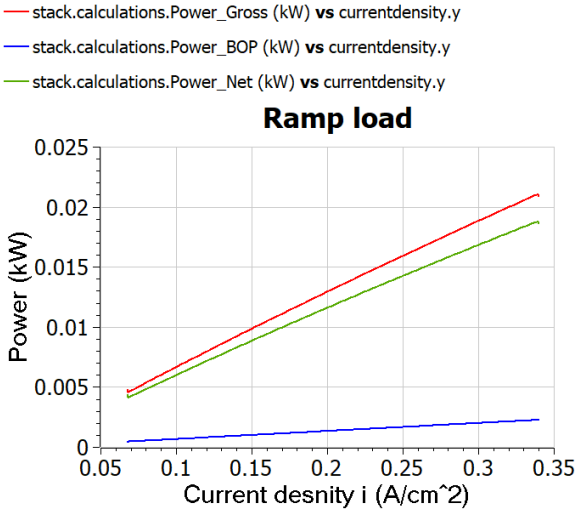


Figure 4.12: Caption for Pi

Figure 4.13: Ramp load analysis

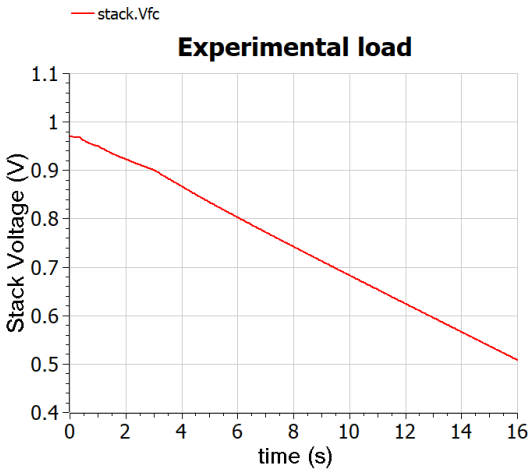
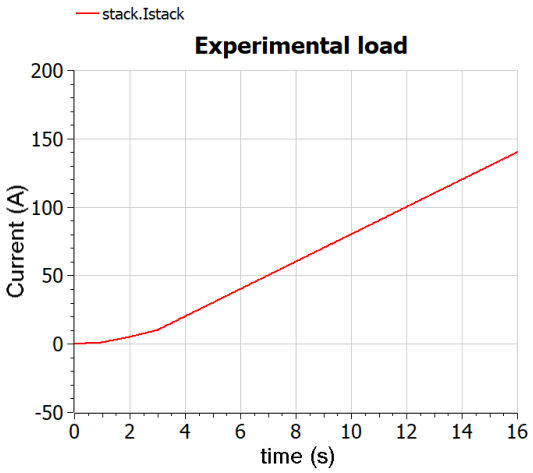


Figure 4.14: Caption for VT



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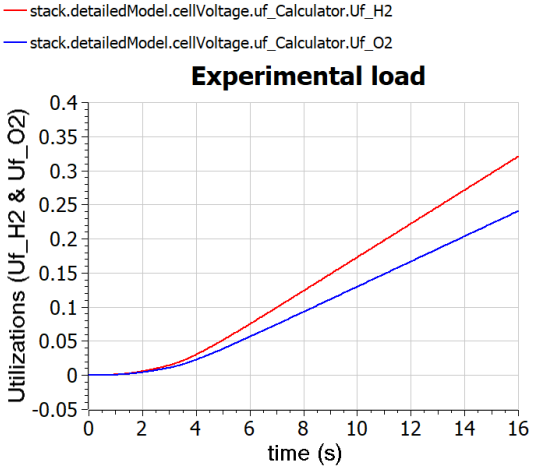


Figure 4.16: Caption for UfT

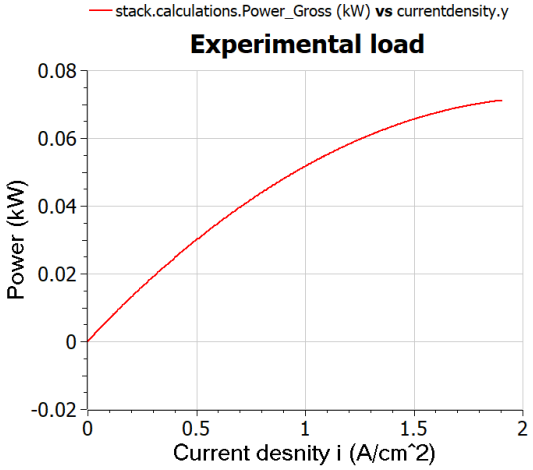


Figure 4.17: Caption for Pi

Figure 4.18: Experimental load and no BoP at $S_1 = 73.6\text{cm}^2$, N = 1, T = 80°C

4.3.3 Polarization curve with surface area 1 and with BoP

Here, we examine how the inclusion of Balance of Plant (BoP) components affects the performance of a PEM fuel cell with the same reference surface area (S1). The response curves illustrates the relationship between voltage and current under these conditions. The presence of BoP components influences the operational factors, such as utilization factor, power consumption, which can impact overall efficiency and performance. This section discusses the impact of the Balance of Plant components on the performance of a PEM fuel cell with a specific reference surface area (S_1). It illustrates how the inclusion of BoP affects the polarization curve, which represents the relationship between the voltage and current of a fuel cell as shown in Figure 4.23. The presence of BoP components typically introduces additional factors into the operation of the fuel cell, such as auxiliary power consumption, which can affect overall efficiency and performance.

4.3.4 Polarization curve with surface area 2 and no BoP

Here, the focus shifts to a PEM fuel cell with a actual surface area (S_2) and the exclusion of BoP components from the analysis. This section's polarization curve (Figure 4.28) show how the fuel cell performs solely based on its intrinsic electrochemical characteristics without the influence of external subsystems like BoP. This can provide insights into the pure performance of the electrochemical surface area under consideration.

4.3.5 Polarization curve with surface area 2 and with BoP

This section combines the conditions of the previous two, examining a PEM fuel cell with actual surface area (S_2) while including the Balance of Plant components. The polarization curve in this scenario would offer a comprehensive view of the fuel cell's performance, taking into account both the electrochemical properties of the larger surface area and the operational impact of BoP components and also serve the realistic operation such as in trucks etc as shown in Figure 4.36. The response for different current demand inputs and the presence of BoP are presented in Figure 4.33. The x-axis represents the demand current (A) to the fuel cell, while the y-axis represents the voltage across the fuel cell (in Volts). This type of curve is useful in understanding the electrical performance of the fuel cell as the current demand varies. In this given

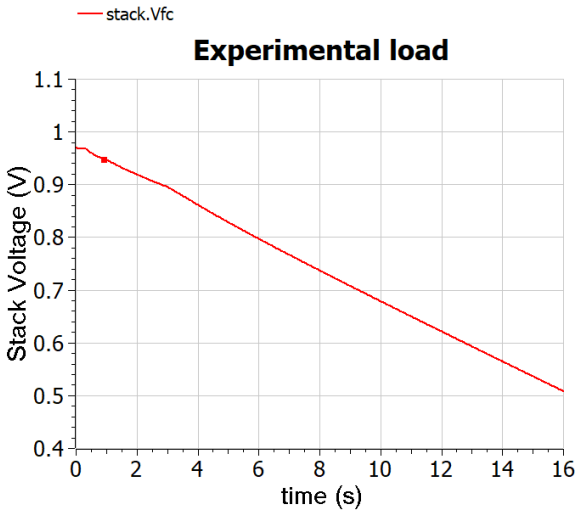
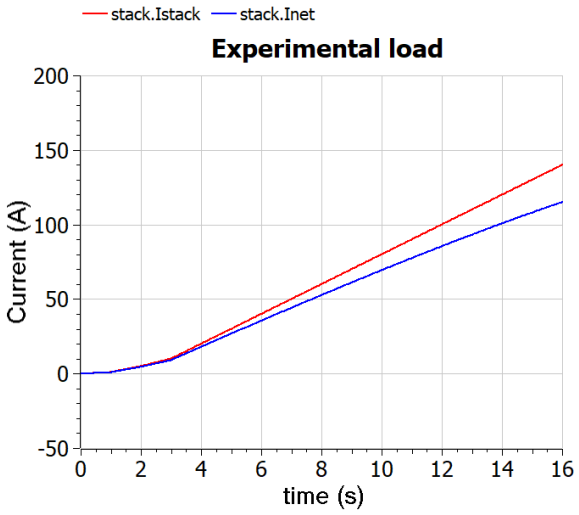


Figure 4.19: Caption for VT



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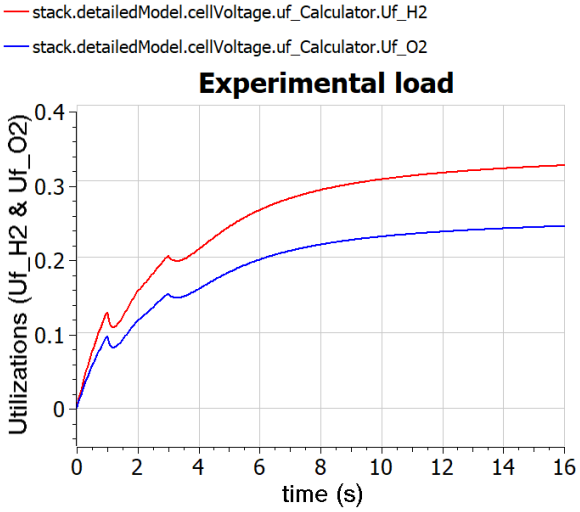

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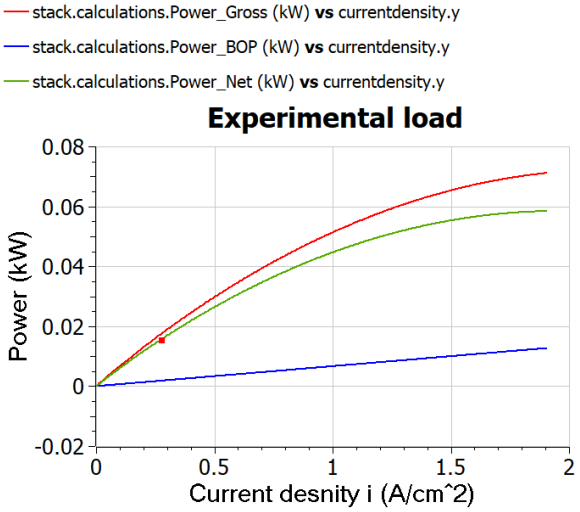
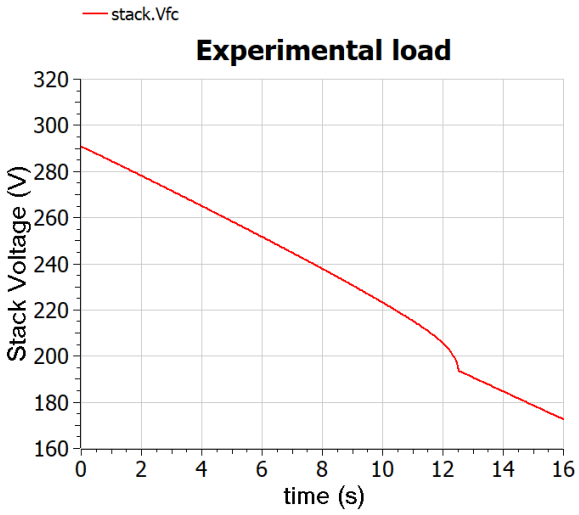


Figure 4.22: Caption for Pi

Figure 4.23: Experimental load and using BoP at $S_1 = 73.6\text{cm}^2$, N = 1



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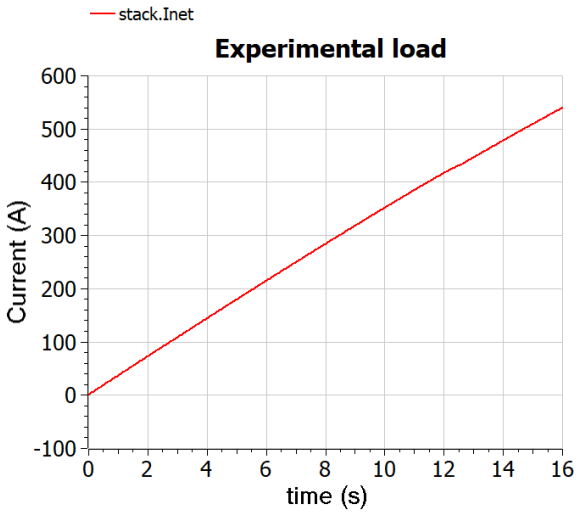

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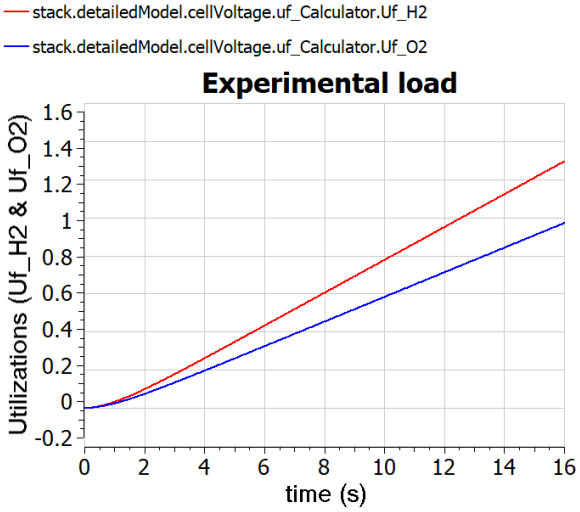


Figure 4.26: Caption for UfT

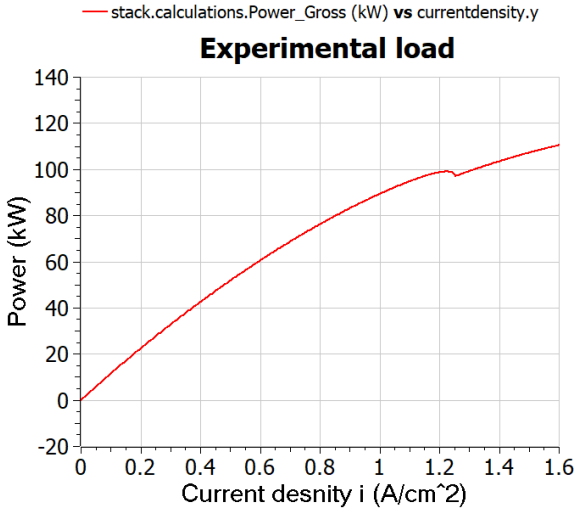


Figure 4.27: Caption for Pi

Figure 4.28: Experimental load and no BoP at $S_2 = 400\text{cm}^2$, N = 300

context, the graph is showing a validation of a model for a larger PEM fuel cell stack intended for heavy-duty applications upon scaling the basic single cell model based on the surface factor (S) (equation 4.1), such as powering trucks, with an output of approximately 275 kW.

$$S = \frac{S_2}{S_1} = \frac{400}{73.6} = 5.434782609 \tag{4.1}$$

where:

S_1: The reference surface area of a single cell, taken as 73.6 $cm2$. This is likely the active area of the electrode where the electrochemical reactions occur.
S_2: The scaled-up surface area, which is 400 $cm2$. This represents an increase in the active area of the electrode, which directly affects the current production capacity of the cell.

This increase in surface area is due to the fact due to the increase in number of cells in the stack which is necessary to meet the power demands from the heavy vehicles (for eg: Trucks). The model cann be easily expanded accordingly from a single cell to a larger number of cells using a cell factor (N) which is given by the equation 4.2.

$$N = \frac{N_2}{N_1} = \frac{300}{1} = 300 \tag{4.2}$$

4.4 Validation at different conditions of operation

It is essential to validate a PEM fuel cell model under various operating situations since actual fuel cells undergo dynamic fluctuations in temperature, pressure, fuel flow, and air flow. A model that has been validated solely at one specific operating point may not effectively forecast performance when faced with these diverse variables, which could potentially result in safety issues, inefficient functioning, or erroneous design choices. By conducting validation tests under various operating situations, you can guarantee that your model accurately reflects the actual behavior of the fuel cell. This will increase your confidence in the model's reliability, enable the development of efficient control techniques, and facilitate optimum design iterations.

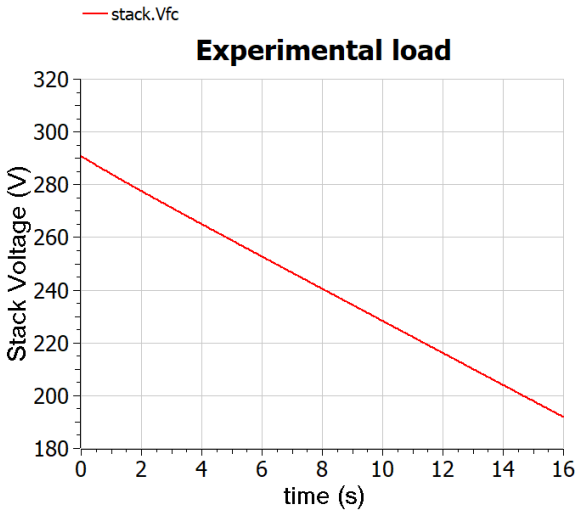
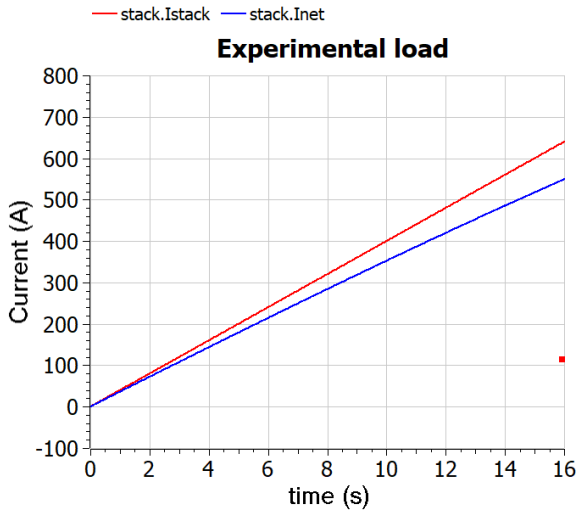


Figure 4.29: Caption for VT



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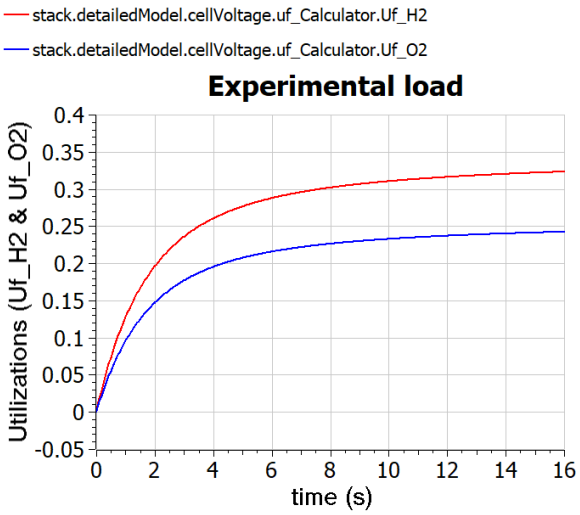

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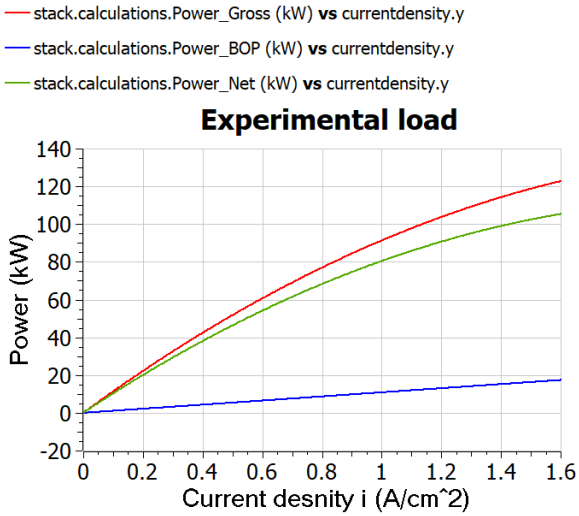

Figure 4.32: Caption for Pi

Figure 4.33: Experimental load and using BoP at $S_2 = 400\text{cm}^2$, N = 300

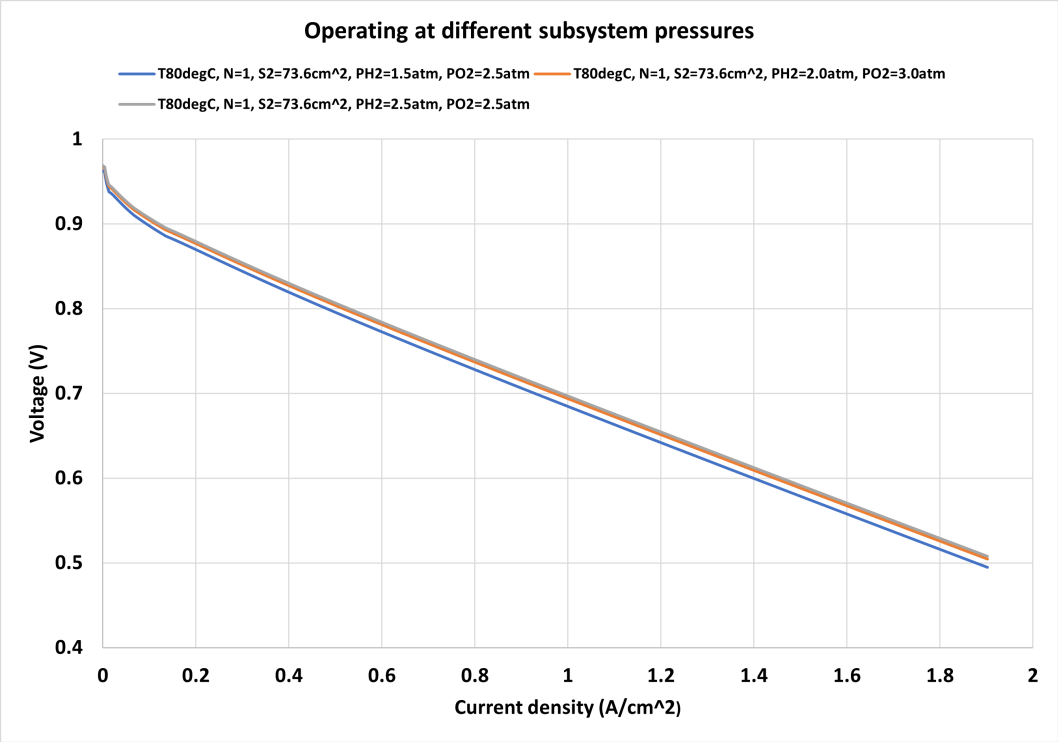

Figure 4.34: Model validation at different pressures

4.4.1 Different subsystem pressures

Figure 4.34 shows the impact of varying operational pressures on the performance of a hydrogen fuel cell, with a focus on the polarization curves that are essential for understanding the electrochemical characteristics of the cell under different conditions. The simulations was carried out for 3 operational variations in the stack pressures, by keeping both pressures at 2.5atm and also by increasing the cathode pressures, illustrating that the fuel cell's efficiency improves as the pressure increases. This improvement is attributed to the enhanced concentration of reactants within the cell due to increased pressure, which facilitates the electrochemical reactions and thus boosts the overall performance of the fuel cell.

The paramters affected are U_f, i_0 & E_n such that:

- Variations in pressure affect the utilization factors of fuel and air within the fuel cell. Higher pressure conditions typically lead to improved utilization factors as reactant concentrations increase, enhancing the efficiency of the electrochemical reactions.

- Changes in pressure can influence the exchange current, which represents the rate of electrochemical reactions at equilibrium. Higher pressures may lead to an increase in exchange current due to the improved availability of reactants at the electrode surface.
- The Nernst voltage, which accounts for the thermodynamic driving force of the electrochemical reactions, is also affected by variations in pressure. Changes in reactant concentrations due to pressure variations can impact the Nernst voltage, affecting cell performance.

The findings reveal that a higher pressure at the cathode, relative to the anode, further improves the cell's performance. This scenario likely improves the diffusion of reactants to the reaction sites and aids in the more efficient removal of products, thereby optimizing the electrochemical process within the cell. It extends the analysis by examining how varying the flow rate of the cathode impacts the cell's performance. Given oxygen's lower cost, it is often used in surplus to ensure an ample supply for the reaction.

These insights underscore the critical role of operational pressures and reactant management in optimizing hydrogen fuel cell performance. By manipulating these parameters, one can significantly influence the efficiency and output of fuel cells, highlighting the importance of precise control over these aspects in fuel cell design and application.

4.4.2 Different temperatures

For a PEM fuel cell, the temperature significantly affects its performance, including parameters such as voltage output, efficiency, and overall power generation capability. The membrane's conductivity rises as temperature increases, resulting in enhanced diffusion of hydrogen protons within the membrane. Consequently, the membrane's resistance decreases, leading to faster electrochemical reactions at higher temperatures, which results in improved voltage output.

In this case the most affected parameters are E_n & i:

- Changes in temperature also affect the Nernst voltage, which reflects the thermodynamic driving force of the electrochemical reactions. Higher temperatures

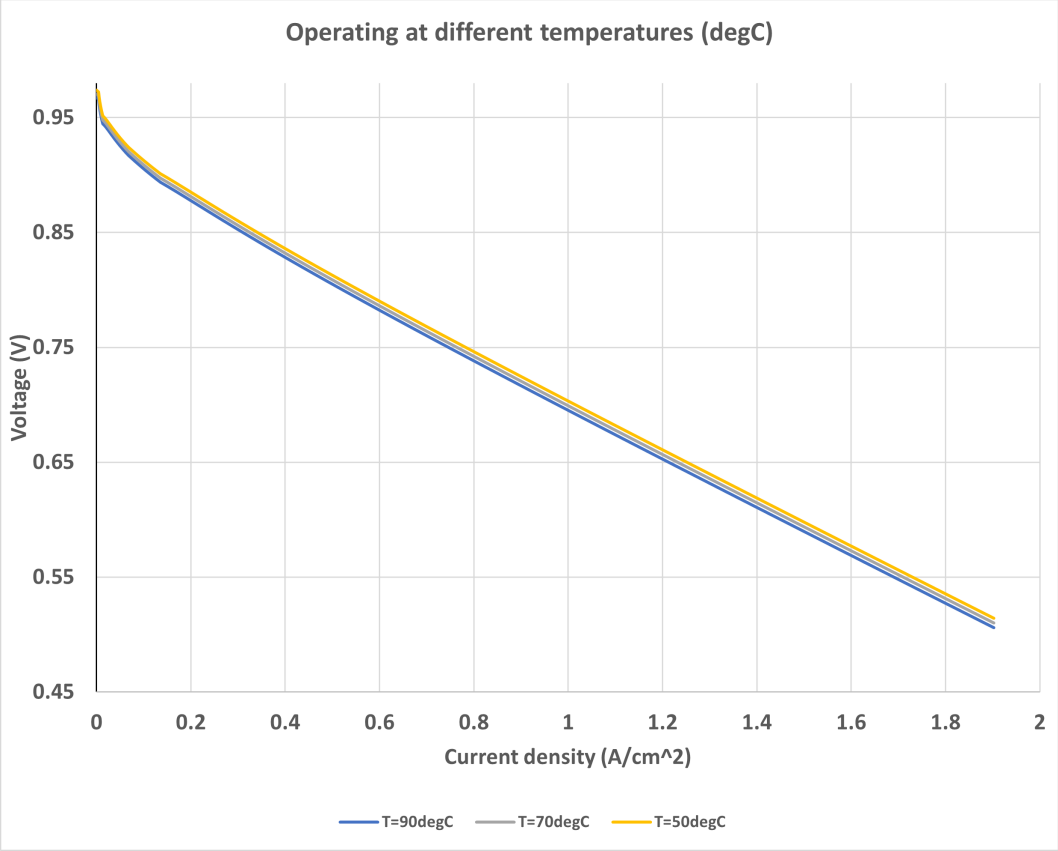

Figure 4.35: Model validation at different temperatures

result in higher Nernst voltages, indicating greater driving forces for the reactions.

- The exchange current density, representing the rate of electrochemical reactions at equilibrium, is influenced by temperature variations. Higher temperatures typically lead to an increase in exchange current density due to the enhanced kinetics of electrochemical reactions.

But, this also leads to generation of water in the cathode, leading to improved hydration of the membrane. As a result, the ionic resistance is decreased. Figure 4.35 illustrates the correlation between temperature and the performance of the stack when operated at different temperatures. It is evident that performance drops as temperature rises indicating the absence of effective water and thermal management which leads to decrease in the performance.

4.5 Key findings and errors

4.5.1 Key findings

Development of a Generic Model: A significant achievement is the development of a generic PEM fuel cell model that is grounded in physical-chemical relationships. This model stands out for its ability to accurately capture the fundamental behaviors of PEM fuel cells, demonstrating the effectiveness of its theoretical foundation.

Modular Structure: The model's construction utilizes a modular approach, enhancing its flexibility and adaptability. This structure not only facilitates future improvements but also enables its integration into different modeling environments, such as Dymola. This versatility is crucial for broadening the model's applicability across various simulation platforms.

Simulation Capabilities: The developed stack model successfully simulates the output of a test bench for a given demand current as load. This capability to replicate real-world operational conditions underscores the model's precision and reliability in predicting fuel cell performance.

Adaptability to Various Manufacturers' Data: By building the model on parametric data, it can accommodate information from multiple manufacturers. This adaptability enhances the model's utility, allowing it to simulate a wide range of fuel cell types and configurations based on diverse specifications.

Response to Load Profiles: The model exhibits precise responses to various load profiles across different numbers of cells and surface areas. The sensitivity of the model to parameter changes further validates its accuracy, showcasing its ability to reflect performance alterations in response to different operational conditions.

4.5.2 Errors and Challenges

Power Demand and BOP Issues: The model struggles to meet the current demand when Balance of Plant (BOP) components are considered, which consume a portion of the generated power. This limitation points to the need for improved energy management within the model.

PI Controller Feasibility: The complexity of the model renders the proposed PI controller for demand management infeasible, leading to issues such as residual functions and cyclic redundancies. This suggests a need for a more sophisticated control strategy.

Experimental Data Alignment: While the experimental data and simulated results are closely aligned, there exists a considerable error range. This approximation indicates the model's high fidelity, although it also highlights the potential for further refinement to enhance accuracy.

Subsystem Robustness: The current model lacks robust subsystems and adequate energy control mechanisms. This limitation restricts the model's ability to fully capture the intricate dynamics of PEM fuel cell operation, suggesting an area for future development.

OpenModelica Challenges: The scarcity of prior work on PEM fuel cells using OpenModelica presents challenges, making the research endeavor more complex. However, this also emphasizes the pioneering nature of the work and its contribution to

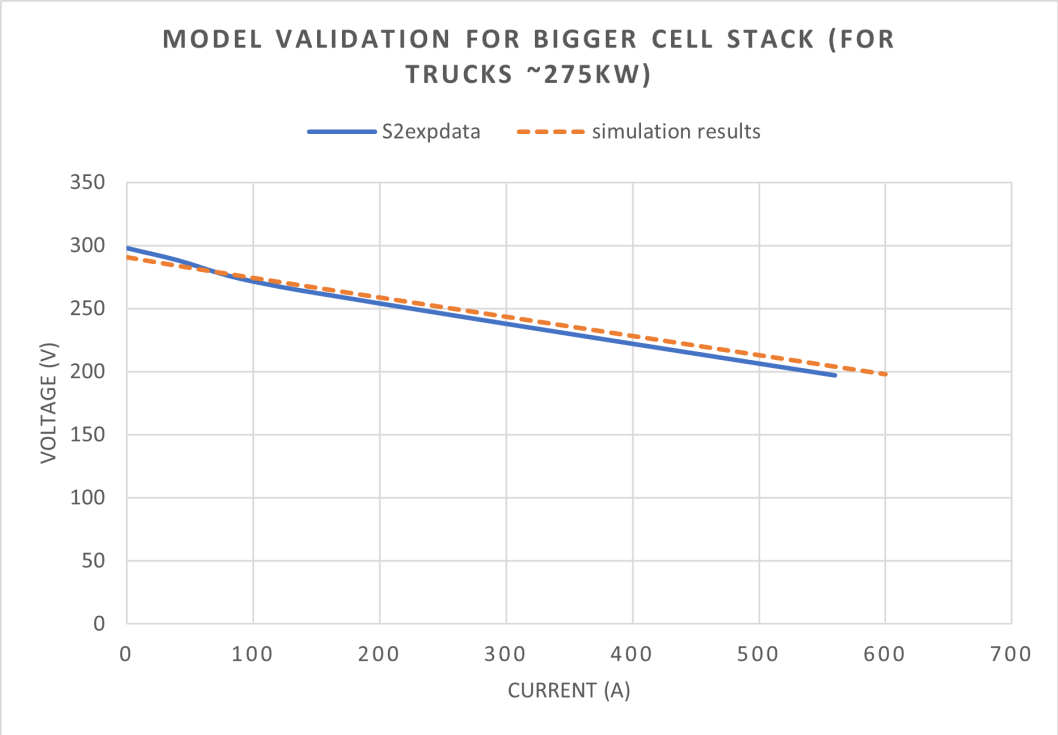

Figure 4.36: Model validation for bigger fuel cell (trucks approximately 275kW)

filling a gap in the field.

5 Conclusion

The thesis provides a thorough examination and results of the modeling and analysis of PEM fuel cells using OpenModelica. The chapter summarizes the substantial progress achieved in comprehending, designing, and simulating PEM fuel cells. This research has enhanced the understanding of PEM fuel cell technology by creating a new and validated model that accurately simulates the dynamic behavior of fuel cells in different operational scenarios, such as step load, ramp load, and experimental load.

The research findings highlight the model's accurate prediction capabilities for the performance of PEM fuel cells, closely matching real-world expectations. By subjecting it to extensive testing using experimental data and known data sheet curves, the model has demonstrated its capacity to accurately represent the key elements of fuel cell operation. This includes accurately accounting for the impact of various load profiles, and the scalability from single cell stacks to larger stacks. This validation not only highlights the precision of the model but also its capacity as a tool for future optimization efforts, due to its modular nature.

Additionally, the study has emphasized the model's flexibility in accurately modeling different application circumstances, hence offering useful insights for the design and optimization of PEM fuel cell systems. The examination of the model under several circumstances, including fluctuations in subsystem pressures, temperatures, and surface areas, both with and without Balance of Plant (BoP) components, has revealed insights into its resilience and adaptability.

In addition to its strengths, this work also acknowledges certain limitations, including inconsistencies in proportional-integral control to meet shifting demand across time. These problems highlight the need for future improvements to the model by integrating more advanced sub-systems to increase water and heat management, humidity control, and other crucial operational aspects.

The model presented is robust and flexible, allowing for improved simulation, design, and optimization of fuel cell systems. The study lays a solid foundation for future investigations by tackling the identified constraints and exploring innovative optimization techniques to enhance the effectiveness and efficiency of PEM fuel cells in different applications.

5.1 Future Scope

The thesis on PEM fuel cell modeling and analysis using OpenModelica can be identified as a basis for various areas for future research, depending on the findings and limits addressed. These paths offer wide range of opportunities to expand upon this existing body of work. Here are possible areas for additional investigation and improvements:

Improvements to the model

- **Integrating Advanced Control Strategies:** In order to overcome the limits of PI control when dealing with time-varying demands, incorporating more advanced control algorithms like Model Predictive Control (MPC) could enhance the model's ability to respond and operate efficiently in dynamic load settings.
- **Improved Water and Thermal Management:** Enhancements in modeling the water and thermal management subsystems could result in more accurate forecasts of fuel cell performance, along with establishing strong control over the humidity of the stack particularly in high-load situations by considering its influence on membrane conductivity and the fuel cell performance.

Incorporating more complex subsystems

- **Comprehensive System Analyses:** Extending the model to include interactions with other components in a complete energy system, such as batteries, supercapacitors, and inverters, could help in designing more efficient and reliable hybrid systems.
- **Multi-domain Modeling:** Moving beyond the current model to incorporate 1D and even multi-domain modeling aspects could enhance the resolution of

simulations, providing deeper insights into the spatial variations within the fuel cell stack.

Real world application and collaboration

- **Cross Collaboration:** Engaging in partnerships with different departments in the company and also with different industries could expedite the practical implementation and experimentation of the model, yielding significant input for subsequent enhancement.
- **Development of Simulation models:** The foundation established by this thesis could lead to the development of advanced simulation models for fuel cell systems of various types, offering valuable resources for researchers, designers, and engineers in the field.

Bibliography

[1] P. Quan, "A study of PEM fuel cell modeling," 5 2021. [Online]. Available: https://rshare.library.torontomu.ca/articles/thesis/A_study_of_PEM_fuel_cell_modeling/14655246

[2] E. I. Ortiz-Rivera, A. Reyes-Hernández, and R. Febo, "Understanding the history of fuel cells," *2007 IEEE Conference on the History of Electric Power*, pp. 117–122, 2007. [Online]. Available: https://api.semanticscholar.org/CorpusID:32696797

[3] C. Spiegel, *PEM Fuel Cell Modeling and Simulation Using Matlab*. Academic Press/Elsevier, 2008.

[4] R. P. O'Hayre, S.-W. Cha, W. G. Colella, and F. B. Prinz, *Fuel cell fundamentals*.

[5] C. Siegel, "High temperature polymer electrolyte membrane fuel cells : modeling, simulation, and segmented measurements /," p. 1 online resource (182 pages). [Online]. Available: http://library.usi.edu/record/961308

[6] S. . Chakraborty, D. . Elangovan, K. . Palaniswamy, A. . Fly, D. . Ravi, D. A. S. . Seelan, T. K. R. A. Rajagopal, V. A. Sadykov, S. Chakraborty, D. Elangovan, K. Palaniswamy, A. Fly, D. Ravi, D. Ashok, S. Seelan, T. Karuppa, and R. Rajagopal, "A review on the numerical studies on the performance of proton exchange membrane fuel cell (pemfc) flow channel designs for automotive applications," *Energies 2022, Vol. 15, Page 9520*, vol. 15, p. 9520, 12 2022. [Online]. Available: https://www.mdpi.com/1996-1073/15/24/9520/htmhttps://www.mdpi.com/1996-1073/15/24/9520

[7] Y. F. Guo, H. C. Chen, and F. C. Wang, "The development of a hybrid pemfc power system," *International Journal of Hydrogen Energy*, vol. 40, pp. 4630–4640, 2015.

[8] J. Andújar and F. Segura, "Fuel cells: History and updating. a walk along two centuries," *Renewable and Sustainable Energy Reviews*, vol. 13, pp. 2309–2322, 2009.

[9] "The gemini program (1962–1966)," https://nssdc.gsfc.nasa.gov/planetary/gemini.html, accessed: 21-September-2022.

[10] H. Abbasi and N. Pourrahmani, "Thermodynamic analysis of a trigeneration system using sofc and hdh desalination unit," *International Journal of Hydrogen Energy*, 2021.

[11] I. Name(s), "Molten carbonate fuel cell," Patent 20 060 204 830A1, 2006.

[12] N. Sammes, R. Bove, and K. Stahl, "Phosphoric acid fuel cells: Fundamentals and applications," *Current Opinion in Solid State and Materials Science*, vol. 8, pp. 372–378, 2004.

[13] A. Hamnett, "Mechanism and electrocatalysis in the direct methanol fuel cell," *Catalysis Today*, vol. 38, pp. 445–457, 1997.

[14] F. M. Alhuwaishel and N. A. Ahmed, "Single stage transformerless microinverter with time sharing operation for pem fuel cell applications," in *2023 IEEE Conference on Power Electronics and Renewable Energy (CPERE)*, 2023, pp. 1–6.

[15] G. C. Catlin, "Pem fuel cell modeling and optimization using a genetic algorithm," 2010. [Online]. Available: https://api.semanticscholar.org/CorpusID:54964063

[16] A. El, M. Aa, A. M. Azmy, and M. Sa, "Dynamic modelling of proton exchange membrane fuel cells for electric vehicle applications," *J Pet Environ Biotechnol*, vol. 5, p. 169, 2014.

[17] L. Vichard, N. Y. Steiner, and D. Hissel, "Existing fuel cell system models: A critical review," Université Bourgogne Franche-Comté (UBFC), Deliverable D3.1 Ref. Ares(2020)7396575 - 07/12/2020, 9 2020, vIRTUAL & physical platform for Fuel Cell System development.

[18] "Plan of software tools," Unknown, Deliverable D2.2 Ref. Ares(2020)3664939 - 10/07/2020, 7 2020, project n° 875087 "VIRTUAL & physical platform for Fuel Cell System development".

[19] X. Z. Yuan, C. Nayoze-Coynel, N. Shaigan, D. Fisher, N. Zhao, N. Zamel, P. Gazdzicki, M. Ulsh, K. A. Friedrich, F. Girard, and U. Groos, "A review of functions, attributes, properties and measurements for the quality control of proton exchange membrane fuel cell components," *J. Power Sources*, vol. 491, p. 229540, Apr. 2021.

[20] M. K. Daletou, J. Kallitsis, and S. G. Neophytides, *6 Materials, Proton Conductivity and Electrocatalysis in High-Temperature PEM Fuel Cells.* New York, NY: Springer New York, 2011, pp. 301–368. [Online]. Available: https://doi.org/10.1007/978-1-4419-5580-7_6

[21] N. Rajalakshmi and K. Dhathathreyan, "Catalyst layer in pemfc electrodes—fabrication, characterisation and analysis," *Chemical Engineering Journal*, vol. 129, no. 1-3, pp. 31–40, 2007.

[22] C.-Y. Wang, "Fundamental models for fuel cell engineering," *Chemical reviews*, vol. 104, no. 10, pp. 4727–4766, 2004.

[23] P. K. Shen, *PEM Fuel Cell Catalyst Layers and MEAs.* London: Springer London, 2008, pp. 355–380. [Online]. Available: https://doi.org/10.1007/978-1-84800-936-3_7

[24] S. Litster and G. McLean, "Pem fuel cell electrodes," *Journal of power sources*, vol. 130, no. 1-2, pp. 61–76, 2004.

[25] A. Kulikovsky, "Quasi-3d modeling of water transport in polymer electrolyte fuel cells," *Journal of the Electrochemical Society*, vol. 150, no. 11, p. A1432, 2003.

[26] *Fuels for Fuel Cells.* John Wiley Sons, Ltd, 2018, ch. 10, pp. 263–321. [Online]. Available: https://onlinelibrary.wiley.com/doi/abs/10.1002/9781118706992.ch10

[27] A. Fly and R. Thring, "Temperature regulation in an evaporatively cooled proton exchange membrane fuel cell stack," *International Journal of Hydrogen Energy*, vol. 37, 05 2015.

[28] A. Akroot, Ekici, and M. Koksal, "Process modeling of an automotive pem fuel cell system," *International Journal of Green Energy*, vol. 16, pp. 1–11, 07 2019.

[29] O. Tremblay, L.-A. Dessaint *et al.*, "A generic fuel cell model for the simulation of fuel cell vehicles," in *2009 IEEE vehicle power and propulsion conference*. IEEE, 2009, pp. 1722–1729.