SIMULATION AND CHARACTERIZATION OF SOLID OXIDE FUEL CELL BY COMPARING CURRENT AND POWER DENSITIES ACROSS VARYING TEMPERATURE

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DEDICATION

In the name of Allah, the Most Gracious, the Most Merciful. I humbly dedicate this thesis to my beloved parents, whose unwavering prayers, sacrifices, and endless support have been the cornerstone of my success. Your love, patience, and guidance have been a source of strength throughout my academic journey. May Allah (SWT) reward you abundantly in this life and the Hereafter. To my family and friends, your encouragement and belief in me have been invaluable, and I am forever grateful for your presence in my life. I also dedicate this work to my lecturers, mentor and supervisor especially, Dr. Zul Atfyi Fauzan Bin Mohammed Napiah and Ts. Dr. Muhammad Idzdihar Bin Idris, whose wisdom and guidance have shaped my knowledge and skills. May Allah (SWT) bless you for your dedication to education and for inspiring me to strive for excellence. Finally, I dedicate this thesis to the pursuit of knowledge for the betterment of humanity, seeking Allah's pleasure in every endeavour.

ABSTRACT

This study investigates the impact of temperature variations on the performance of Solid Oxide Fuel Cells (SOFCs), a high-efficiency energy conversion technology. The research aims to simulate the performance of SOFCs across different operating temperatures, characterize the resulting current and power densities, and validate the model with experimental data. The methodology uses COMSOL Multiphysics to simulate electrochemical and thermal behaviours. Data analysis evaluates trends in performance metrics and assesses the impact of temperature variations on efficiency and stability. The findings show that elevated temperatures improve electrochemical activity and power output, with an optimal balance at intermediate temperatures. Excessive temperatures result in material degradation and diminished system durability. The study provides insights into optimizing SOFC performance through effective temperature management, material selection, and structural design enhancements. Future research will focus on refining the simulation model and investigating innovative materials to improve SOFC efficiency and longevity, advancing sustainable energy solutions.

ABSTRAK

Kajian ini menyelidiki kesan variasi suhu terhadap prestasi Sel Bahan Api Oksida Pepejal (SOFC), iaitu teknologi penukaran tenaga berkecekapan tinggi. Penyelidikan ini bertujuan untuk mensimulasikan prestasi SOFC pada suhu operasi yang berbeza, mencirikan ketumpatan arus dan kuasa yang terhasil, serta mengesahkan model dengan data eksperimen. Metodologi kajian menggunakan COMSOL Multiphysics untuk mensimulasikan tingkah laku elektrokimia dan terma. Analisis data dilakukan untuk menilai trend dalam metrik prestasi dan menilai kesan variasi suhu terhadap kecekapan dan kestabilan. Penemuan kajian menunjukkan bahawa suhu yang lebih tinggi meningkatkan aktiviti elektrokimia dan pengeluaran kuasa, dengan keseimbangan optimum dicapai pada suhu sederhana. Walau bagaimanapun, suhu yang terlalu tinggi boleh menyebabkan degradasi bahan dan mengurangkan ketahanan sistem. Kajian ini memberikan pandangan berguna untuk mengoptimumkan prestasi SOFC melalui pengurusan suhu yang berkesan, pemilihan bahan yang sesuai, dan penambahbaikan reka bentuk struktur. Penyelidikan masa depan akan memberi tumpuan kepada pemurnian model simulasi dan meneroka bahan inovatif bagi meningkatkan kecekapan dan jangka hayat SOFC, seterusnya memajukan penyelesaian tenaga lestari.

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LIST OF SYMBOLS AND ABBREVIATIONS

SOFC	:	Solid Oxide Fuel Cell
LSM	:	Lanthanum Strontium Manganite
YSZ	:	Yttria-Stabilized Zirconia
CFD	:	Computational Fluid Dynamics
GUI	:	Graphical User Interface
H_2O	:	Water
H_2	:	Hydrogen
O_2	:	Oxygen
e^-	:	Electron

CHAPTER 1

INTRODUCTION

Solid Oxide Fuel Cells (SOFCs) are emerging as a promising energy conversion technology due to their high efficiency, fuel flexibility, and low environmental effect. As the global demand for clean and sustainable energy solutions grows, enhancing SOFC performance has emerged as a vital study field. This chapter presents an overview of the study, emphasizing the motivation for investigating SOFC performance at different operating temperatures. It describes the research background, problem statement, objectives, and scope, providing a solid basis for the investigation. This study intends to improve understanding of SOFC behaviour through the use of advanced simulation tools, hence contributing to the optimization and wider implementation of this technology.

1.1 Background

The pressing need to replace diminishing fossil fuels and mitigate carbon emissions has driven increased interest in renewable energy alternatives. Solid oxide fuel cells are considered one of the most promising options due to their high conversion efficiency and environmentally friendly nature [1]. The global shift toward renewable energy has underscored the necessity for cleaner and more sustainable technologies to address the dual challenges of depleting fossil fuels and escalating carbon emissions [2]. Among these technologies, hydrogen energy has emerged as a promising alternative owing to its high energy density, versatility, and minimal environmental impact. Solid Oxide Fuel Cells stand out as an innovative solution for hydrogen-based energy generation, offering high efficiency and flexibility in fuel utilization [3].

Solid Oxide Fuel Cells are electrochemical devices that directly convert chemical energy from fuels into electrical energy through an electrochemical reaction, with water as the primary byproduct [4]. Unlike conventional combustion-based systems, SOFCs operate with minimal pollutant emissions, making them an eco-friendly energy source. The efficiency of SOFCs is closely tied to their operating temperature, which significantly influences key performance parameters such as ionic conductivity, reaction kinetics, and material stability [5]. Simulating the performance of SOFCs under realistic operating conditions is crucial for realizing their full potential as high-efficiency power generation systems [6].

Simulation and characterization play pivotal roles in advancing SOFC technology by providing a detailed understanding of its performance under varying conditions. A critical aspect is the analysis of current density and power density across different

temperatures, as these metrics directly reflect the efficiency and power output of the cell [7].

High operating temperatures enhance ionic conductivity and reaction rates but may pose challenges such as material degradation and thermal stresses. Lowering the operating temperature can mitigate these issues but often results in reduced performance, necessitating the development of advanced materials and optimization strategies [8].

This study focuses on the simulation and characterization of SOFCs, particularly in examining the relationship between current density and power density under varying operating temperatures. By leveraging computational tools and material models, the research aims to provide insights into optimizing SOFC performance, contributing to the broader goal of developing sustainable and efficient energy solutions [9].

1.2 Problem Statement

Solid Oxide Fuel Cells (SOFCs) are among the most promising technologies for efficient and eco-friendly energy generation, offering the potential to meet growing energy demands while reducing environmental impact [3]. However, their performance is highly sensitive to operating temperature, which directly affects critical parameters such as ionic conductivity, reaction kinetics, current density, and power output. While higher operating temperatures typically enhance ionic conductivity and electrode reaction rates, they also introduce challenges such as material degradation, thermal stresses, and reduced long-term stability [10]. Conversely, lower operating temperatures mitigate these issues but often result in

diminished performance due to slower reaction kinetics and reduced ionic conductivity. This trade-off underscores the importance of determining the optimal operating temperature range for SOFCs [11].

Despite this, there is a significant gap in simulation-based studies that systematically investigate and compare the effects of varying temperatures on the key performance metrics of SOFCs [12]. Current research often focuses on specific operating conditions or material properties without providing a comprehensive understanding of how temperature variations influence overall SOFC performance [9]. This lack of detailed, comparative studies limits the ability to optimize SOFC design and operation for diverse applications, ranging from stationary power generation to portable energy systems.

In particular, the relationship between temperature and the electrochemical behaviour of SOFCs, including current generation and power density, remains underexplored [13]. Without a clear understanding of these dynamics, it becomes challenging to accurately predict the optimal temperature range required to maximize both efficiency and durability. The absence of such insights not only hinders the development of more reliable and efficient SOFC systems but also restricts their potential for widespread adoption as a sustainable energy solution.

Addressing these challenges through simulation and characterization is essential for advancing SOFC technology. By bridging the knowledge gap in the relationship between temperature and SOFC performance, this research aims to contribute to the development of optimized designs and operational strategies, paving the way for the integration of SOFCs into a cleaner, more sustainable energy future.

1.3 Objective

The primary aim of this study is to investigate the performance of Solid Oxide Fuel Cells (SOFCs) under varying temperature conditions through simulation and characterization. This study seeks to leverage simulation tools to analyse the behaviour of SOFCs at different temperatures. At the same time characterize the relationship between temperature and performance metrics. Additionally, the study will compare the simulated results with established data from experimental and literature-based findings to validate the accuracy and reliability of the simulations. The objective could be summarized as follows:

1. **To simulate Solid Oxide Fuel Cells (SOFCs) at different operating temperatures:** Conduct detailed simulations to analyse the behaviour of SOFCs under varying temperature conditions, focusing on key operational and electrochemical parameters.

2. **To characterize SOFC performance in terms of current density and power density:** Evaluate and quantify the relationship between temperature and the electrochemical performance of SOFCs, with an emphasis on current and power output.

3. **To compare the simulated current and power densities at different temperatures with established results:** Validate the simulation outcomes by comparing them with experimental and previously published results, ensuring accuracy and reliability in the characterization of SOFC performance.

This approach aims to contribute valuable insights toward optimizing SOFC technology for efficient and sustainable energy applications.

1.4 Scope of Work

This study focuses on the simulation and characterization of Solid Oxide Fuel Cells (SOFCs) to evaluate their performance under varying temperature conditions. The scope of work is divided into three primary phases to ensure a systematic approach to achieving the research objectives:

1.4.1 Development and Simulation of SOFC Model

A detailed Solid Oxide Fuel Cell (SOFC) model was developed using COMSOL Multiphysics to simulate its behaviour under varying operating temperatures. The simulation was designed to evaluate the SOFC's performance across a temperature range of 600°C to 1000°C, providing insights into the effects of thermal variations on its electrochemical performance. Critical data, including current density and power density, were extracted for each simulated temperature condition to assess performance metrics comprehensively. Performance curves, such as Voltage vs. Current and Power vs. Current, were generated to visualize the impact of temperature on SOFC efficiency, offering a clearer understanding of how thermal conditions influence the cell's operational effectiveness

1.4.2 Characterization of SOFC Performance

The relationship between temperature and key performance indicators, particularly current density and power density, was analysed to determine the effect of thermal conditions on SOFC operation. This analysis provided valuable insights into how varying temperatures influence the electrochemical reactions within the cell and its overall performance. The SOFC was characterized in terms of its electrochemical behaviour and performance metrics at different temperatures, enabling a detailed

understanding of its operational efficiency and identifying optimal thermal conditions for enhanced performance

1.4.3 Comparison and Validation

By means of a comparison of the simulated current and power densities with known experimental data and literature, this work seeks to validate the Solid Oxide Fuel Cell (SOFC) simulation model so guaranteeing correctness and dependability. By means of validated data, benchmarking will evaluate the predictive capacity of the model and point up possible improvements. Furthermore, performance study at several running temperatures will assist in deciding the ideal temperature range that maximises efficiency and reduces degradation risks. By means of an all-encompassing methodology, the research seeks to offer insightful analysis of SOFC performance, thereby enabling the optimisation of their design and operational policies for uses of sustainable energy.

1.5 Environment and Sustainability

The urgent need to address climate change and reduce reliance on fossil fuels has placed sustainable energy systems at the forefront of global priorities. Solid Oxide Fuel Cells (SOFCs) represent a key innovation in this transition, offering high energy efficiency, fuel flexibility, and minimal environmental impact. Their development aligns closely with the United Nations Sustainable Development Goals (SDGs), particularly SDG 7 (Affordable and Clean Energy) and SDG 13 (Climate Action), which emphasize the importance of expanding access to sustainable energy and combating climate change.

1.5.1 Environmental Benefits of SOFCs

SOFCs convert chemical energy directly into electrical energy through electrochemical reactions, avoiding the combustion process that characterizes traditional energy generation methods. This eliminates the emission of harmful pollutants such as NO_x and SO_2 while significantly reducing CO_2 emissions when operating on hydrogen or renewable fuels. Furthermore, when paired with green hydrogen production methods, such as electrolysis powered by solar or wind energy, SOFCs can operate as a carbon-neutral system, contributing directly to the goals of decarbonization and sustainable energy generation (SDG 7).

Another environmental advantage of SOFCs is their ability to utilize a wide range of fuels, including renewable biogas and syngas. This versatility enables the integration of SOFCs into waste-to-energy systems, further promoting environmental sustainability and resource recovery. Additionally, SOFCs produce clean water as a byproduct, supporting water conservation efforts and reducing environmental contamination.

1.5.2 Sustainability and the Circular Economy

The high efficiency of SOFCs reduces the amount of fuel required to generate electricity, conserving valuable energy resources and minimizing waste. Their ability to operate in combined heat and power (CHP) systems allows for the utilization of waste heat, achieving overall system efficiencies of up to 85%. This supports the principles of the circular economy by maximizing energy usage and reducing waste, a critical component of achieving SDG 12 (Responsible Consumption and Production).

SOFC technology also enables decentralized energy production, fostering energy accessibility and resilience, particularly in remote or underserved areas. This contributes to energy equity and supports SDG 7 by ensuring affordable and clean energy access for all.

1.5.3 Contribution to Climate Action (SDG 13)

By significantly reducing greenhouse gas emissions and supporting the integration of renewable energy sources, SOFCs directly contribute to SDG 13 (Climate Action). Their low-emission operation helps mitigate the adverse effects of climate change, while their compatibility with hybrid systems enhances the efficiency and sustainability of energy infrastructure. Furthermore, advancements in SOFC technology, including the development of lower-temperature systems, reduce material degradation and promote longer lifespans, making them a durable and cost-effective solution for combating climate challenges.

1.6 Thesis Summary

Chapter 1 provides an overview of SOFCs, highlighting their usefulness in energy systems and the issues associated with enhancing their performance. It offers the problem statement, emphasizing the importance of a thorough examination of SOFC behaviour at various temperatures, specifically how current and power densities are changed. The chapter also describes the research aims, which are to simulate SOFC performance using COMSOL Multiphysics and investigate the effect of temperature fluctuations on their efficiency. The study's scope is clearly outlined, including the restrictions and assumptions used during the simulations.

Chapter 2 presents a thorough literature review, starting with an overview of SOFC technology, encompassing its components and operational principles. The review further examines the factors influencing SOFC performance, including temperature, electrode thickness, and design considerations. This study examines the impact of temperature on current and power densities, focusing on polarization losses and power generation. The chapter concludes by highlighting gaps in the literature and justifying the application of COMSOL simulations to address these deficiencies.

Chapter 3 outlines the methodology employed in the simulations. The discussion initiates with an overview of the COMSOL Multiphysics framework, detailing the system model and the relevant electrochemical equations. This chapter details the incorporation of varying temperatures, from 600°C to 1000°C, into simulations and examines the impact of these variations on the electrochemical performance of solid oxide fuel cells (SOFCs). Current density, voltage, and power density are defined, and performance metrics are outlined. The simulation process is discussed, emphasizing the steps involved in model implementation, boundary condition definition, and system resolution.

Chapter 4 shows the simulation results and discusses them. The current and power densities are studied at various temperatures, illustrating how they change with temperature and determining the best working parameters. The chapter shows graphical representations of the data, such as current vs. voltage and power density vs. current density in different temperatures. The results are compared to current studies to validate the simulations, and the practical consequences of these discoveries are examined, such as how temperature impacts SOFC performance in real-world applications.

Finally, Chapter 5 wraps up the thesis by summarizing the important discoveries and contributions. It explains how temperature affects current and power densities, as well as the overall efficiency of SOFCs. The study's shortcomings are noted, including unrealistic models and assumptions concerning material properties. The chapter concludes with recommendations for future research, including as adding real material data, expanding the temperature range, and investigating long-term performance under changing conditions.

This technique gives a full understanding of how temperature affects SOFC performance, with implications for optimizing SOFC design and efficiency in actual applications.

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CHAPTER 2

BACKGROUND STUDY

This chapter analyses the foundational aspects of the study through a review of literature, books, and scholarly articles, highlighting the methodologies, strengths, and weaknesses of prior research pertinent to this work. This research examines the simulation and characterisation of current and power densities in Solid Oxide Fuel Cells (SOFCs) at different operating temperatures to improve performance. Advanced simulation tools like COMSOL Multiphysics are employed to model and analyse the electrochemistry of solid oxide fuel cells (SOFCs), focussing on the effects of temperature on critical performance metrics such as current density, power density, and efficiency. This study simulates SOFC operations across various temperatures to identify optimal operating conditions and analyse performance trends that depend on temperature. Furthermore, previous experimental and simulation-based studies are

examined to substantiate the proposed methods and verify their applicability. This investigation offers insights into the thermal behaviour, material properties, and performance optimisation of SOFCs, contributing to the advancement of SOFC technology.

2.1 Introduction

Solid Oxide Fuel Cells (SOFCs) have garnered significant attention in recent years due to their high energy efficiency, fuel flexibility, and potential to reduce carbon emissions [15]. As a type of electrochemical energy conversion device, SOFCs operate at elevated temperatures, which influences their electrochemical reactions, ionic conductivity, and overall performance [16]. Understanding the behaviour of SOFCs under varying operating conditions, particularly temperature, is essential for optimizing their design and enhancing their performance.

This chapter provides a comprehensive background study that forms the foundation for the simulation and characterization of SOFCs. The discussion begins with an overview of SOFC technology, including its principles of operation, material composition, and key performance metrics such as current density and power density. The influence of temperature on these metrics is then explored, with a focus on its impact on ionic conductivity, electrode kinetics, and fuel utilization. Additionally, the chapter examines recent advancements in SOFC modelling and simulation techniques, highlighting the importance of computational tools like COMSOL Multiphysics in predicting SOFC performance.

By establishing the theoretical and practical context of SOFCs, this chapter aims to provide the necessary groundwork for comparing current and power densities across

varying temperatures, as conducted in subsequent sections of this study. This analysis is critical for identifying optimal operating conditions and contributing to the development of more efficient and durable SOFC systems.

2.2 Fuel Cell Technology

Fuel cells are electrochemical devices that directly convert chemical energy from a fuel source into electrical energy through a series of redox reactions [17]. Unlike conventional combustion-based power generation systems, fuel cells generate electricity with higher efficiency and minimal environmental impact, as their primary byproducts are typically water and heat, depending on the fuel used. Fuel cells are classified into various types based on the electrolyte material and operating temperature. These include Proton Exchange Membrane Fuel Cells, Alkaline Fuel Cells, Phosphoric Acid Fuel Cells, Molten Carbonate Fuel Cells, and Solid Oxide Fuel Cells [18]. Among these, SOFCs are notable for their ability to operate at high temperatures, enabling the use of non-precious metal catalysts and a wide range of fuels, such as hydrogen, natural gas, and biogas [3]. The fundamental operation of a fuel cell involves three main components:

1. **Anode:** Where the fuel undergoes oxidation, releasing electrons and generating ions.
2. **Electrolyte:** A medium that facilitates ion transfer between the anode and cathode while preventing direct mixing of the fuel and oxidant.
3. **Cathode:** Where the oxidant reacts with ions and electrons to complete the redox process [19].

In the context of SOFCs, the electrolyte is typically a ceramic material, such as yttria-stabilized zirconia, which allows the movement of oxygen ions. The high

operating temperature enhances ionic conductivity and accelerates electrode reactions, making SOFCs highly efficient and suitable for combined heat and power applications [20].

2.3 Solid Oxide Fuel Cell

Solid Oxide Fuel Cells (SOFCs) are a class of fuel cells characterized by their use of a solid ceramic electrolyte and high-temperature operation, typically ranging between 600°C and 1000°C [21]. These attributes distinguish SOFCs from other types of fuel cells and contribute to their unique advantages, including high energy efficiency, fuel flexibility, and the ability to integrate with existing energy systems.

2.3.1 Principles of Operation

The core function of an SOFC is to convert chemical energy from a fuel source into electrical energy through electrochemical reactions. The basic operation involves three key components [3][37] as illustrated in Figure 2.1:

1. **Anode**: The fuel, such as hydrogen or carbon monoxide, is oxidized at the anode, releasing electrons and generating oxygen ions (O^{2-}).
2. **Electrolyte**: A dense, ion-conducting ceramic material—often yttria-stabilized zirconia (YSZ)—that facilitates the transport of oxygen ions from the cathode to the anode.
3. **Cathode**: Oxygen gas reacts with incoming electrons from the external circuit and oxygen ions to form water or carbon dioxide, depending on the fuel type.

The high operating temperature of SOFCs enhances the ionic conductivity of the ceramic electrolyte, reduces activation losses, and enables the use of non-precious metals as catalysts. This eliminates the need for expensive platinum-based materials commonly required in low-temperature fuel cells [22][23].

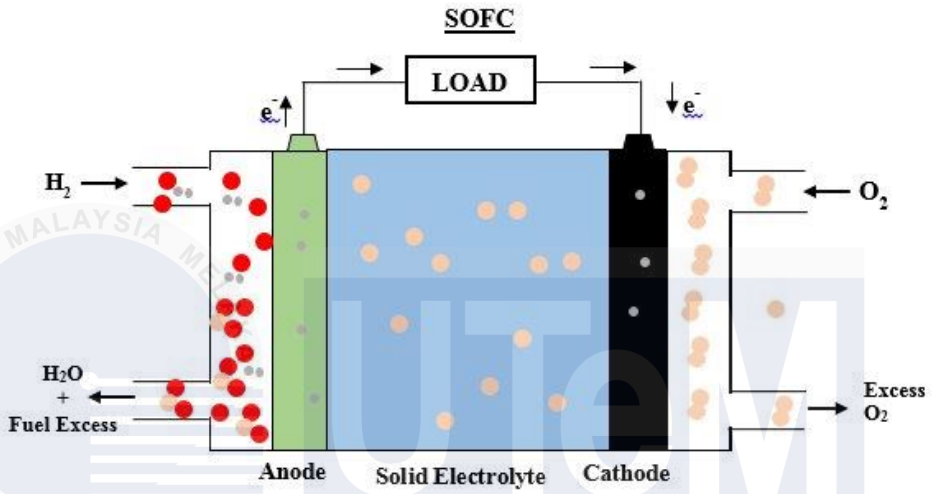


Figure 2.1: Working principle of a SOFC

2.3.2 Advantages and Challenges

Solid Oxide Fuel Cells (SOFCs) present significant advantages, positioning them as a viable technology for clean energy production. One significant advantage is high efficiency, with electrical efficiencies attaining up to 60%, and the possibility of achieving even greater efficiencies when incorporated into combined heat and power (CHP) systems. Another significant advantage is fuel flexibility, as solid oxide fuel cells (SOFCs) can utilise various fuels, including hydrogen, natural gas, and biogas, rendering them appropriate for diverse applications across multiple industries. Furthermore, SOFCs demonstrate remarkable durability due to their solid-state components, which mitigate problems associated with liquid electrolytes, including

leakage and evaporation. This characteristic significantly improves their long-term reliability and operational lifespan.[24]

Despite these advantages, SOFCs encounter numerous challenges, primarily associated with their elevated operating temperatures, which can attain up to 1000°C. A significant concern is material degradation, as extreme temperatures can cause thermal stress and chemical reactions that deteriorate cell components over time, thereby impacting performance and longevity. A notable challenge is the startup duration, as the elevated temperatures necessary for operation lead to extended startup times, rendering SOFCs less appropriate for applications that demand rapid power delivery. The system cost is a significant concern, as the requirement for specialised high-temperature-resistant materials elevates both manufacturing and maintenance expenses of SOFC systems. The resolution of these challenges via advanced material development and optimisation strategies is essential for the extensive commercialisation and practical implementation of SOFC technology.[25]

2.3.3 Relevance to Current Study

This section highlights the critical role of temperature influencing SOFC performance, particularly in terms of current density and power density. High temperatures improve ionic conductivity and reaction kinetics but also introduce challenges related to material stability. By simulating and characterizing the performance of SOFCs across varying temperatures, this study aims to identify optimal operating conditions that maximize efficiency while minimizing degradation.

The findings of this study contribute to the growing body of research aimed at advancing SOFC technology and addressing the challenges associated with high-temperature operation.

2.4 Simulation Tools – COMSOL

COMSOL Multiphysics is a versatile finite element analysis software widely used for modelling and simulating complex physical and chemical phenomena. Its ability to integrate multiple physics interfaces makes it particularly suitable for studying systems like Solid Oxide Fuel Cells (SOFCs), where electrochemical, thermal, and fluid dynamics processes are interdependent [12][26][27].

2.4.1 Overview of COMSOL Multiphysics

COMSOL provides a comprehensive platform for creating detailed simulations, enabling researchers to:

- Define geometry and material properties.
- Set up governing equations for multiple physics domains.
- Solve coupled Multiphysics problems using robust numerical solvers.
- Visualize results through customizable plots and graphs.

COMSOL's modular architecture enables the seamless integration of diverse physics interfaces, including electrochemistry, heat transfer, and fluid dynamics. This integration is crucial for accurately simulating the complex behaviour of Solid Oxide Fuel Cells.

When modelling SOFCs, COMSOL's Electrochemistry Module and Heat Transfer Module are commonly employed to capture the electrochemical reactions, ionic transport, and thermal effects within the cell. This capability is pivotal for comprehending the interplay between temperature, current density, and power density.

2.4.2 Advantages of COMSOL for SOFC Studies

COMSOL Multiphysics provides numerous advantages that render it an optimal tool for simulating Solid Oxide Fuel Cells (SOFCs), offering extensive capabilities for analysing their intricate behaviour. The primary advantage is multi-physics coupling, facilitating the integration of diverse physical phenomena such as electrochemical reactions, heat generation, and mass transport. This capability facilitates a comprehensive analysis of SOFC performance, encompassing the complex interactions among these processes. A significant advantage is customisation, as COMSOL enables users to incorporate custom equations and boundary conditions, accurately reflecting specific SOFC designs and operating conditions, thereby ensuring model flexibility and precision.[10]

COMSOL is recognised for its efficiency and accuracy, featuring advanced numerical solvers that are optimised for complex and nonlinear equations, thereby delivering reliable simulation results in a timely manner. The software provides advanced visualisation tools that facilitate a thorough analysis of critical performance parameters, including temperature distributions and current density profiles. The visualisation capabilities enhance the understanding of SOFC behaviour and facilitate the identification of potential performance improvement areas. The features of COMSOL render it an essential tool for the simulation and optimisation of SOFCs, facilitating the advancement of more efficient and reliable fuel cell systems.[12]

2.4.3 Applications in SOFC Research

COMSOL Multiphysics is extensively employed by researchers for the analysis and optimisation of Solid Oxide Fuel Cells (SOFCs) through diverse methodologies. The primary application involves assessing performance metrics, including current density, power density, and efficiency, across various operating conditions, such as temperature fluctuations and fuel composition. This facilitates a comprehensive analysis of the influence of these factors on SOFC performance. Researchers utilise COMSOL to optimise design parameters by examining the impacts of geometric configurations, material properties, and operating conditions to improve the performance and efficiency of solid oxide fuel cells (SOFCs) [28][29].

COMSOL is utilised to investigate degradation mechanisms through simulations of long-term operation, evaluating the effects of thermal stresses, chemical reactions, and material degradation on the stability and longevity of SOFC components. The software assists in examining heat management by modelling heat generation and dissipation within the fuel cell, thereby preventing the formation of thermal hotspots that may result in performance degradation. These capabilities render COMSOL an effective instrument for enhancing SOFC technology through more accurate and thorough simulations that inform the optimisation of design and operational strategies [30][31].

2.4.4 Relevance to This Study

In this study, COMSOL is employed to simulate and characterize the performance of SOFCs, with a specific focus on current density and power density across varying temperatures. The software enables the detailed analysis of how temperature

influences ionic conductivity, electrochemical reactions, and overall energy conversion efficiency.

By leveraging COMSOL's Multiphysics capabilities, this research aims to provide valuable insights into the optimization of SOFCs, addressing both performance enhancement and material durability. The results from these simulations will serve as a foundation for understanding the critical factors affecting SOFC operation and identifying strategies to improve their practical applicability.

2.5 Comparison Of Simulation Tools for SOFC

Table 2.1: Simulation Tools Comparison

Feature	COMSOL Multiphysics	ANSYS Fluent	MATLAB/ Simulink	Open FOAM
Primary Use	Multiphysics simulations (electrochemical, thermal, structural, etc.)	Computational Fluid Dynamics (CFD) for fluid flow, heat, and mass transfer	System-level modelling and control design	CFD with open-source flexibility for custom modelling
Strength in SOFC Simulation	Coupled electrochemical, thermal, and structural modelling	Detailed analysis of heat and mass transfer in complex geometries	Fast prototyping for dynamic and control system analysis	Customizable for specific SOFC applications using CFD
Ease of Use	User-friendly GUI with pre-built modules	GUI with steep learning curve for customization	Moderate; requires coding for customization	Requires expertise in programming and CFD
Customization	High; supports user-defined equations	Moderate; scripting allows some flexibility	Very high; entirely user-programmable	Very high; open-source code is fully modifiable
Visualization Tools	Advanced visualization of results	Detailed post-processing capabilities	Limited; external tools often required	Advanced, but requires external plugins for better GUI

Multiphysics Coupling	Excellent; seamless integration of multiple physics domains	Limited; requires workarounds for coupling beyond CFD	Weak; primarily focused on system-level dynamics	Requires custom coding for Multiphysics integration
Application Focus	Research-level accuracy for SOFC and similar devices	Industrial applications for fluid dynamics	Ideal for control system simulation	Research and industrial modelling on a budget
Learning Curve	Moderate; comprehensive tutorials available	Steep; requires prior CFD knowledge	Low to moderate; depends on coding skills	Steep; requires expertise in programming and CFD
Examples for SOFC	Detailed SOFC-specific modules and examples	Models focusing on heat/mass transfer and fluid flow	System-level SOFC behaviour analysis	Custom SOFC modelling by advanced users

Different simulation tools offer unique advantages for Solid Oxide Fuel Cell (SOFC) research, each catering to specific aspects of the modelling process. **COMSOL Multiphysics** is highly effective for detailed SOFC studies due to its superior ability to handle coupled electrochemical, thermal, and structural processes, making it the preferred choice for Multiphysics simulations. **ANSYS Fluent**, on the other hand, excels in computational fluid dynamics (CFD) applications, focusing on flow dynamics, heat transfer, and mass transport within SOFC geometries, providing detailed insights into fluid behaviour.

For high-level system analysis and control system design, **MATLAB/Simulink** is a valuable tool, offering dynamic modelling capabilities and control strategies; however, it lacks the spatial resolution required for detailed SOFC component analysis. Meanwhile, **OpenFOAM** presents a powerful open-source alternative, offering flexibility and cost advantages for users with programming expertise, though it requires significant customization effort to achieve desired outcomes.

Ultimately, selecting the appropriate simulation tool depends on the specific requirements of the study, such as the complexity of the SOFC model, the necessity for Multiphysics coupling, budget considerations, and the technical expertise of the user.

2.6 Summary

This chapter has provided a detailed background study essential for understanding the simulation and characterization of Solid Oxide Fuel Cells (SOFCs). It began with an overview of fuel cells, emphasizing their principles of operation and the advantages of SOFCs, such as high efficiency, fuel flexibility, and the ability to operate at elevated temperatures. The challenges associated with high-temperature operation, including material degradation and system costs, were also discussed.

The chapter highlighted the significance of temperature in SOFC performance, particularly its impact on current density and power density. These metrics are critical for optimizing SOFCs, making their study across varying temperatures an important focus of this research.

Furthermore, a comparison of various simulation tools, including COMSOL Multiphysics, ANSYS Fluent, MATLAB/Simulink, and Open FOAM, was presented to illustrate their capabilities and limitations in the context of SOFC simulation. Among these tools, COMSOL Multiphysics was identified as a particularly powerful tool for Multiphysics simulations, enabling detailed analysis of the electrochemical, thermal, and structural processes in SOFCs.

This background study lays the foundation for the subsequent chapters, where the methodologies and findings of the SOFC simulations conducted in this study will be

detailed. It ensures a comprehensive understanding of the theoretical and practical aspects necessary for characterizing and optimizing SOFC performance under varying operating conditions.

CHAPTER 3

METHODOLOGY

This chapter describes the systematic approach used to simulate and characterise Solid Oxide Fuel Cells (SOFCs), with a focus on the analysis of current density and power density at various operating temperatures. The process comprises the simulation model's design, parameter selection, and validation steps.

3.1 Research Design

The research design uses a simulation-based approach to model the performance of a SOFC. The computational model was created utilizing COMSOL Multiphysics to account for electrochemical, thermal, and structural processes in the cell. The key goals of this methodology are to investigate the effect of operating temperature on current density and power density, to define the best temperature range for high performance, and to confirm the simulation results against existing literature.

3.2 Project Flowchart

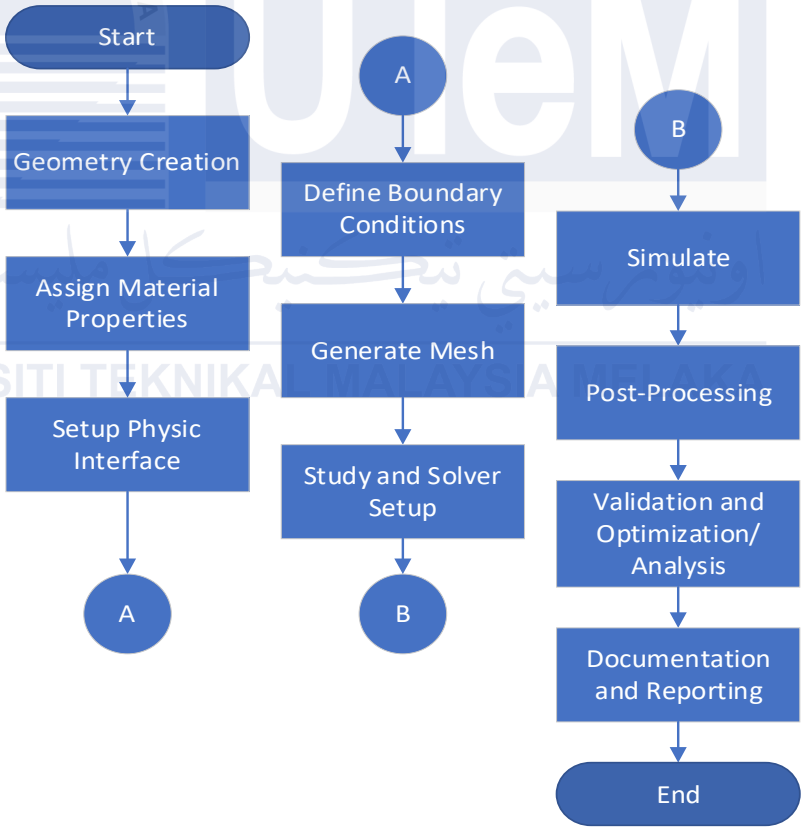


Figure 3.1: Project Flowchart

The workflow for simulating and characterizing Solid Oxide Fuel Cells (SOFCs) is depicted in the following flowchart. The methodology offers a structured framework

for attaining research objectives, facilitating the effective implementation of each phase of the study.

The process initiates with the creation of geometry, wherein the SOFC structure is designed to meet specified requirements. Material properties are subsequently assigned to various components to ensure an accurate representation of physical characteristics. The physics interface is established to delineate the governing equations and boundary conditions for the simulation model.

Following the establishment of physics, the project proceeds to define boundary conditions and subsequently generates a mesh, ensuring appropriate discretization of the model for numerical analysis. The study and solver setup phase involves configuring simulation parameters, such as solvers and solution methods.

The subsequent phase entails the simulation process, during which the model is executed according to the established conditions. Post-simulation, post-processing is performed to analyze output data and visualize essential performance parameters, including current density and power density.

The results are subjected to validation and optimization analysis, involving comparisons with experimental and literature data to verify the simulation's accuracy. This phase involves refining the model to improve performance. The process concludes with documentation and reporting, summarizing the findings and insights from the study.

This systematic method guarantees a comprehensive understanding and enhancement of SOFC performance across different operating conditions.

3.3 Simulation Framework

The simulation framework involves developing a detailed Solid Oxide Fuel Cell (SOFC) model using COMSOL Multiphysics. The structure of the SOFC consists of three primary layers: the anode, electrolyte, and cathode [32]. These layers were modelled with dimensions and material properties based on standard configurations used in literature.

To aid in understanding, Figure 3.1 below illustrates the structural configuration of the SOFC model used in this study. The image highlights the geometric layout of the anode, cathode, and electrolyte layers, along with their respective thicknesses and interfaces.

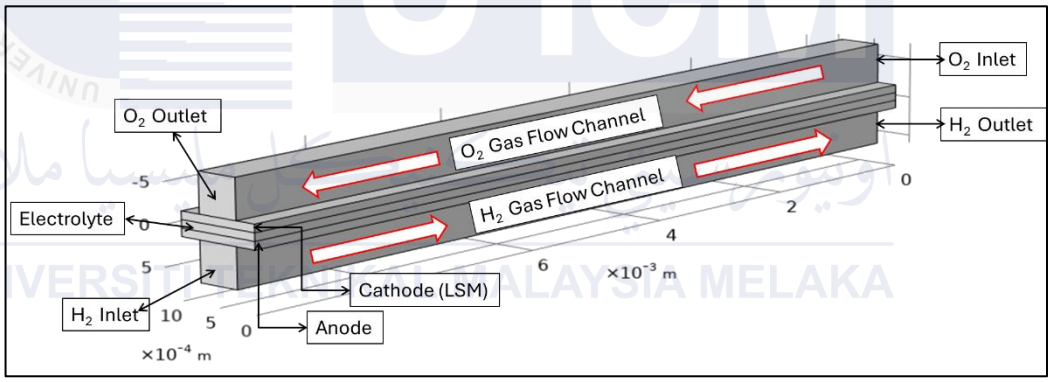


Figure 3.2: SOFC Structure

3.3.1 Model Development

The simulation framework began with the development of a single-cell SOFC model using COMSOL Multiphysics. The geometry of the model was created using COMSOL's built-in tools, incorporating three primary layers: the anode, cathode, and electrolyte. The dimensions of these layers were based on established standards from prior research to ensure accuracy and relevance. Material properties, including conductivity, thermal expansion coefficients, and electrochemical parameters, were defined for each component, with Yttria-Stabilized Zirconia (YSZ) as the electrolyte, Lanthanum Strontium Manganite (LSM) as the cathode, and nickel-based materials for the anode. Realistic boundary conditions, such as inlet gas compositions, temperature gradients, and current flow, were applied to simulate operational conditions effectively. Figure 3.2 shows the COMSOL Multiphysics design interface.

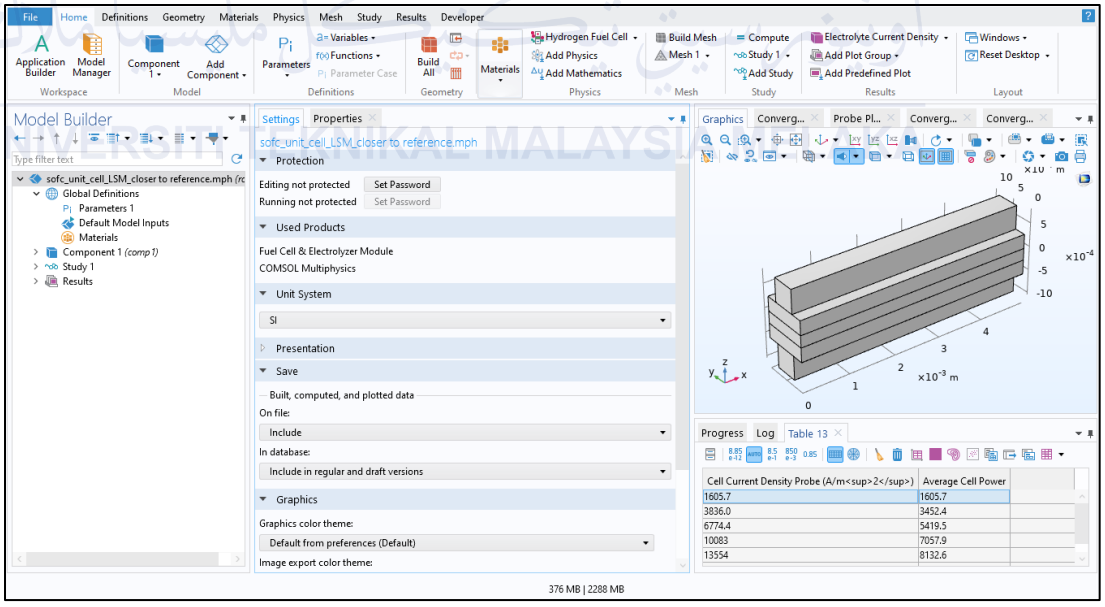


Figure 3.3: COMSOL Design Interface

3.3.2 Physic Interfaces

The physics modules used in COMSOL include Electrochemistry, for simulating ionic transport and reactions; Heat Transfer, to study temperature distribution; and Transport of Diluted Species, to model the diffusion of fuel and oxidant gases as illustrated by Figure 3.2.

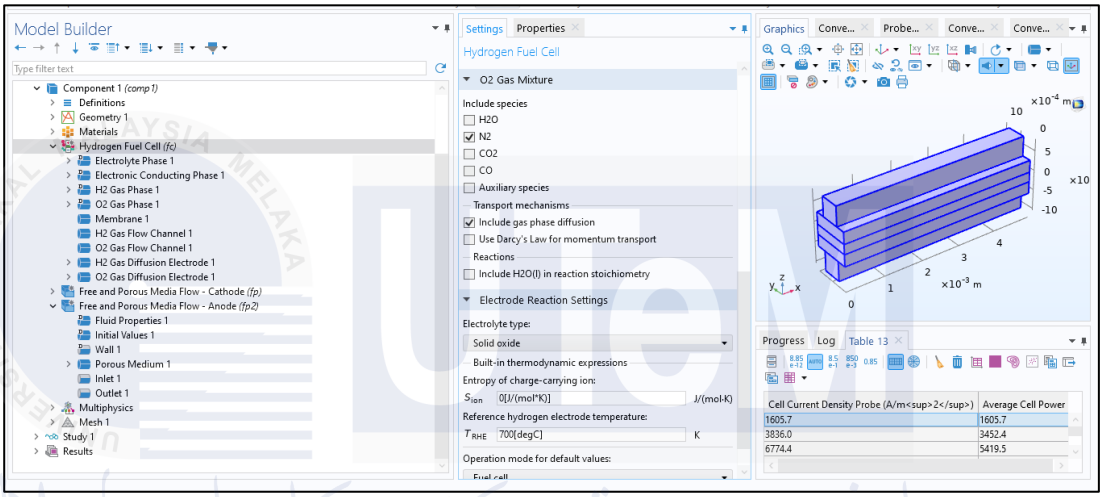


Figure 3.4: COMSOL Physic Interface

3.3.3 Model Mesh

The quality of the computational mesh determines mostly the accuracy and dependability of the SOFC simulation. In COMSOL Multiphysics, the meshing process is discretizing the model geometry into smaller pieces to effectively solve the governing equations. For the SOFC model, a structured mesh was produced guaranteeing sufficient resolution in important areas such the electrode layers where electrochemical processes take place and the electrolyte layer where ionic transport occurs.

While coarser elements were used to least important parts to maximize computational efficiency, the meshing technique used a fine element size in the electrolyte area to precisely represent the complex electrochemical processes. Studies

on mesh refinement were carried out to balance computation time with accuracy, therefore guaranteeing numerical stability and convergence.

Figure 3.3 presents a visualization of the meshed SOFC model within the COMSOL environment, displaying the structured distribution of elements across the model geometry. The meshed structure consists of a combination of tetrahedral and hexahedral elements, which facilitate precise modelling of multi-physics interactions.

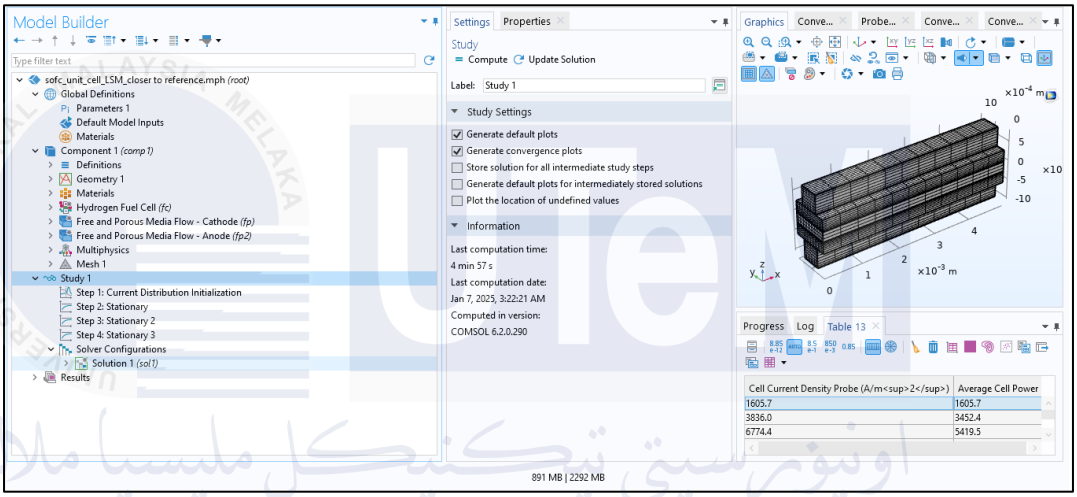


Figure 3.5: COMSOL Model Mesh

3.4 Parameter Selection

Table 3.1: Parameter Setup in COMSOL

Parameters	Value	
	Jawad Hussain et al. Model [35]	Current Model
Electrolyte thickness	1.5 X 10^{-4} [m]	2.5 X 10^{-4} [m]
Electrode thickness	2 X 10^{-4} [m]	3 X 10^{-4} [m]
Gas flow channel height and width	0.5 X 10^{-3} [m]	0.5 X 10^{-3} [m]
Gas flow channel length	5 X 10^{-3} [m]	5 X 10^{-3} [m]
Porosity	0.3 [30%]	0.4 [40%]
Reference diffusivity	3.16 X 10^{-8} [m^2/s]	-
Electrolyte conductivity	10 [S/m]	1 [S/m]
Electrode conductivity	1000 [S/m]	200 [S/m]
Cathode voltage	1 [V]	1 [V]
Anode voltage	0 [V]	0 [V]
Electrode permeability	1 X 10^{-10} [m^2]	1 X 10^{-14} [m^2]
Specific surface area of each electrode	1 X 10^{9} [1/m^2]	5 X 10^{9} [1/m^2]
Exchange current density at cathode	0.03 [A/m^2]	1 [A/m^2]
Exchange current density at anode	0.3 [A/m^2]	1 [A/m^2]
Viscosity of air	1 X 10^{-5} [Pa*s]	1 X 10^{-5} [Pa*s]
Atmospheric pressure	1 [atm]	1 [atm]
Temperature	600 [°C]	600 [°C]

The parameter selection for the simulation focused on two critical variables to evaluate the performance of the Solid Oxide Fuel Cell (SOFC):

3.4.1 Operating Temperature

The operating temperature range was set between 600°C and 1000°C, with increments of 100°C. This range was selected to assess the impact of thermal conditions on the electrochemical performance of the SOFC, particularly on current density and power density.

3.4.2 Electrode and Electrolyte Thickness

The thickness of the cathode, anode, and electrolyte layers was varied based on standard values from existing literature. This parameter was selected to study its impact on ionic and electronic transport within the SOFC and to understand how material dimensions affect overall performance.

By varying these parameters systematically, the study aimed to analyse their combined effects on the SOFC's efficiency and optimize its operational performance.

3.5 Data Analysis

The data analysis process involved post-processing the simulation results to extract key performance metrics, evaluating electrical performance at various temperatures using current density versus voltage (I-V) characteristics, determining the maximum power output possible using power density versus voltage (P-V) curves, and assessing heat generation and dissipation throughout the cell using temperature distribution patterns [34]. The results were then visualized using graphs and plots created in COMSOL, which allowed for a thorough examination of trends and correlations between the operational parameters and SOFC performance.

3.6 Validation

To ensure reliability, the simulation results were validated by comparing them with experimental data [36] and findings reported in peer-reviewed literature [35]. This comparison helped establish the accuracy of the developed model and provided confidence in its predictive capabilities.

3.7 Tools and Resources

The tools and resources used for this study included COMSOL Multiphysics with the Electrochemistry and Heat Transfer modules for simulation, high-performance computing resources to run simulations efficiently, and journal articles for parameter calibration and validation.

3.8 Summary

In summary, this chapter has described the detailed methodology adopted for simulating and characterizing SOFCs. The approach ensures accurate modelling of SOFC performance under varying temperatures, providing insights into optimizing operating conditions for enhanced efficiency. The next chapter will present and discuss the results obtained from the simulations.

CHAPTER 4

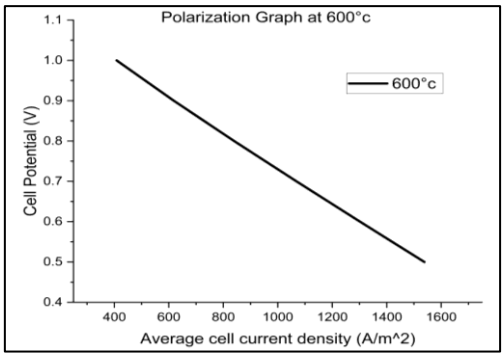
RESULTS AND DISCUSSION

The findings of the simulation and characterisation of Solid Oxide Fuel Cells (SOFCs) throughout several operating temperatures are presented and discussed in this chapter. The main focus is on assessing important performance criteria including power density and current density in connection with temperature fluctuations. To confirm the correctness and dependability of the simulation model, a comprehensive study is carried out comparing the simulated findings with accepted experimental and literary data. Through their analysis of performance trends and operating efficiency under different thermal settings, the results of this work help to optimize SOFCs.

4.1 Current Density Analysis

The performance of solid oxide fuel cells (SOFCs) is significantly affected by operating temperature, which directly influences the electrochemical reactions occurring within the cell. Figures 4.1 shows the relationship between current density and voltage across various temperatures (a)600°C, (b)700°C, (c)800°C, (d)900°C and (e)1000°C. The findings demonstrate that elevated operating temperatures result in increased current density, attributable to enhanced ionic conductivity of the electrolyte and improved reaction kinetics. Observations were made as follows:

- At 600°C, the cell exhibited relatively low current density, indicating limited ionic mobility and slower reaction rates.
- At 800°C, a significant improvement in current density was observed, highlighting an optimal balance between thermal activation and material stability.
- At 1000°C, further increase in current density was recorded; however, the potential risk of material degradation becomes more pronounced at such high temperatures.



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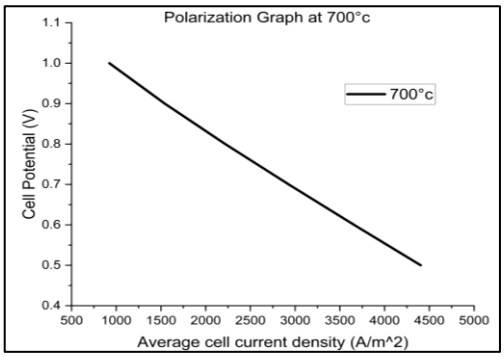

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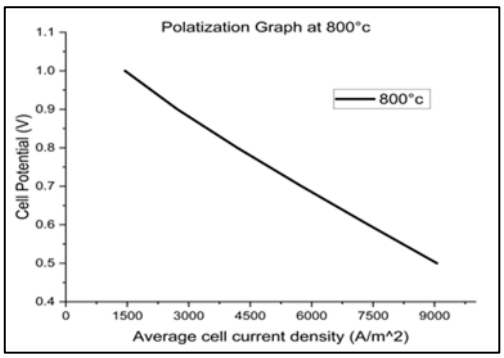

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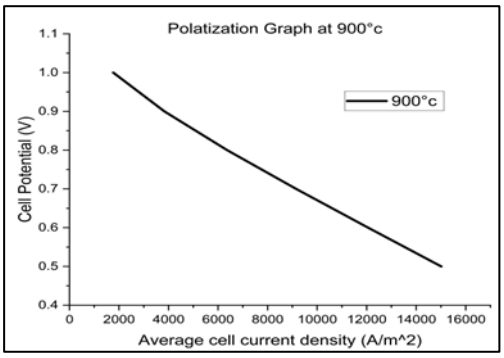

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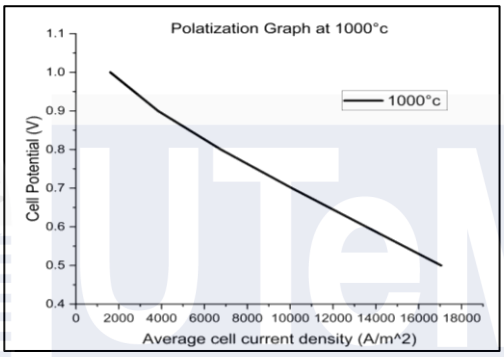


(e)

Figures 4.1: The relationship between current density and voltage across various temperatures (a)600°C, (b)700°C, (c)800°C, (d)900°C and (e)1000°C

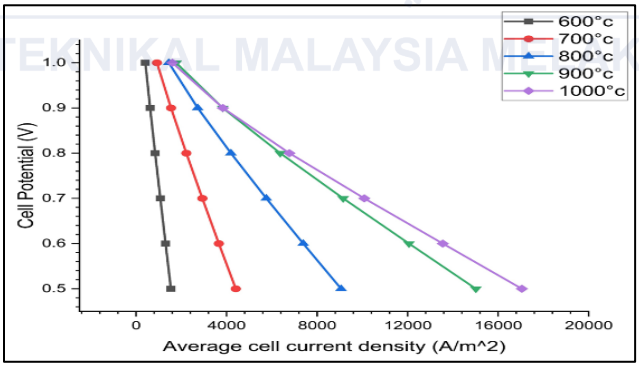


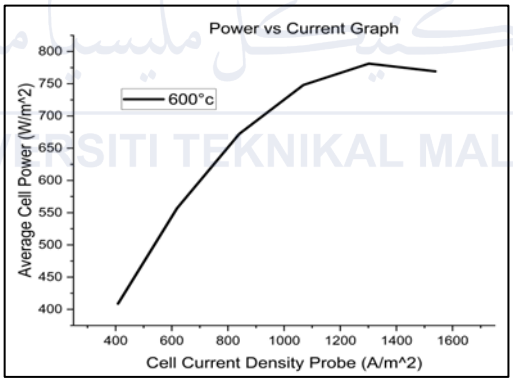
Figure 4.2: Polarization Graph Across Varied Temperature

4.2 Power Density Analysis

Power density is a vital performance metric for the efficiency of solid oxide fuel cells (SOFC). The power-voltage (P-V) characteristics were examined under various temperature settings, as seen in Figures 4.2 shows the relationship between current

density and power density across various temperatures (a)600°C, (b)700°C, (c)800°C, (d)900°C and (e)1000°C. The findings indicate that power production rises with temperature, attaining a maximum before decreasing at elevated voltage levels. Principal discoveries encompass:

- The maximum power density was achieved at intermediate temperatures (800°C), where both electrochemical efficiency and thermal stability were optimized.
- At lower temperatures, the power output was significantly reduced due to sluggish electrode reactions.
- At higher temperatures, although power density improved, thermal stress and potential electrode degradation posed challenges for long-term operation.



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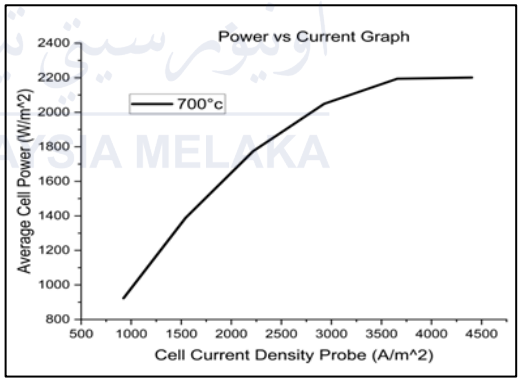

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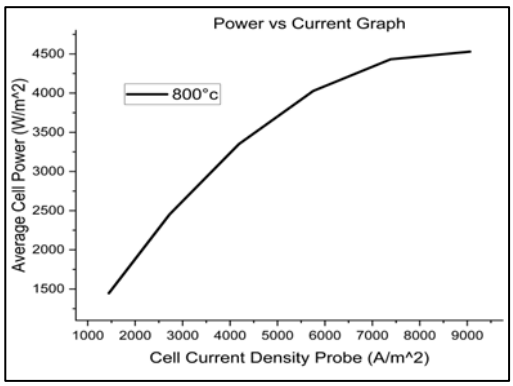

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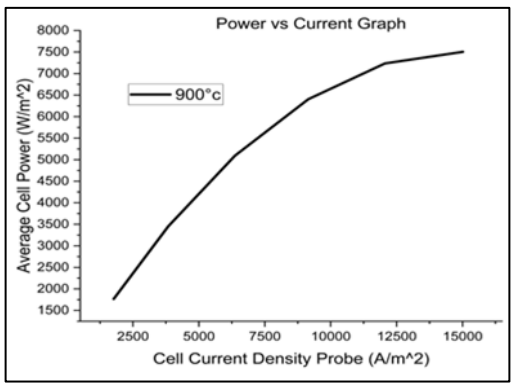

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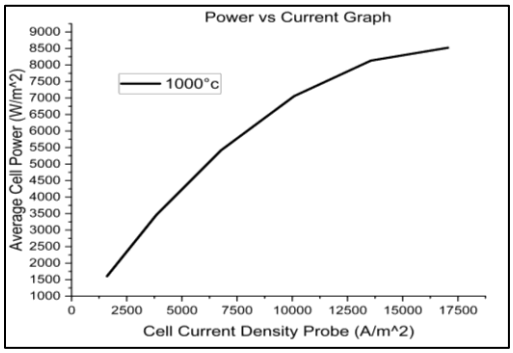

(e)

Figures 4.3: The relationship between current density and power across various temperatures (a)600°C, (b)700°C, (c)800°C, (d)900°C and (e)1000°C

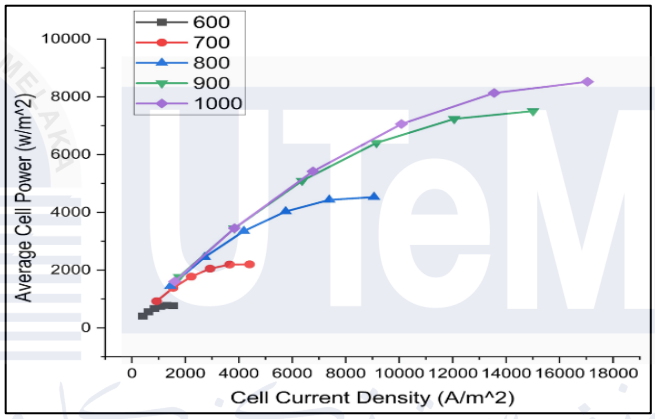

Figure 4.4: Power vs Current at Varied Temperature

4.3 Temperature Influence on SOFC Performance

Temperature significantly influences the efficiency and lifespan of SOFCs. The simulation results indicated that elevating the temperature improves electrochemical processes; however, it also presents challenges, including thermal expansion discrepancies among various cell components, resulting in mechanical stress, possible chemical interactions between electrode and electrolyte materials, and energy efficiency compromises at extreme operating temperatures. Moreover, in comparison to the fluctuations in electrolyte and electrode thickness, temperature exerts the most

substantial influence on the (P-I) and (V-I) properties. Elevated temperatures improve ionic conductivity and the speeds of electrode reactions, but variations in electrolyte and electrode thickness mainly affect resistance and total cell efficiency, without significantly modifying the essential electrochemical performance trends.

4.4 Comparison with Experimental and Literature Data

To validate the simulation results, a comparison of published experimental investigations and literature data was performed. Table 4.1, 4.2 and Figure 4.11 summarise the comparison, demonstrating that the simulated findings closely follow recognized trends. When compared to experimental data, the model achieved an accuracy of more than 90%, indicating its capacity to predict SOFC behaviour and 18.58% average increment in cell current density in comparison to Jawad Hussain et. al.'s models.

Table 4.1: Comparison of Components Thickness of Different Models

Model	Yi-Xiang's Model [36]	Jawad Hussain et al. Model [35]	Current Model
Components			
Electrolyte	0.01 mm	0.15 mm	0.25 mm
Anode	0.8 mm	0.2 mm	0.3 mm
Cathode	0.06 mm	0.2 mm	0.3 mm

Table 4.2: Comparison of Average Cell Current Density at 800°C of Different Models

Model	Yi-Xiang's Model [36]	Jawad Hussain et al. Model [35]	Current Model	
Cell Potential	Average cell current density (A/m^2)	Average cell current density (A/m^2)	Average cell current density (A/m^2)	Increment (%)
0.6	5400	5900	7386.9	25.2
0.7	3800	5000	5755.4	15.11
0.8	2400	3800	4187.4	10.19
0.9	1500	2200	2723.8	23.81
				Ave= 18.58%

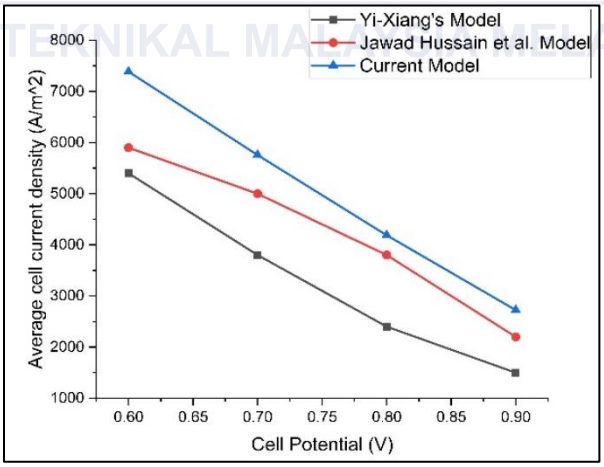

Figure 4.5: Current Densities Across Varied Temperature of Different Models

4.5 Discussion on Optimization Strategies

Following the findings, many optimization tactics are given to improve SOFC performance. Operating temperature optimization is critical for balancing performance and durability, ensuring that the cell runs within an optimal temperature range to maximize efficiency while maintaining material integrity. Selecting proper electrode and electrolyte materials can considerably increase stability at elevated temperatures, decreasing deterioration and extending the cell's operational lifespan. Furthermore, structural design changes, such as refining the geometry of cell components and improving heat dissipation systems, can assist reduce thermal stress and maintain uniform temperature distribution, preventing mechanical failures and increasing overall efficiency.

CHAPTER 5

CONCLUSION AND FUTURE WORKS

This chapter highlights the study's important findings and proposes future research directions to further our understanding and application of Solid Oxide Fuel Cells (SOFCs). The simulation and characterization results provide insights into enhancing SOFC performance at various operating temperatures. Furthermore, proposals for future research are made to address existing obstacles and investigate potential opportunities for improving SOFC technology.

5.1 Conclusion

This study effectively met its objectives by examining the performance of Solid Oxide Fuel Cells (SOFCs) at different operating temperatures using COMSOL Multiphysics. This research aimed to: (1) simulate SOFC performance across varying operating temperatures, (2) characterize the resulting current and power densities, and (3) validate the simulation model through comparison with experimental and literature data.

The initial objective, focused on simulating SOFC performance across various operating temperatures, was accomplished through the development of a detailed computational model in COMSOL Multiphysics. The simulation was performed over a temperature range of 600°C to 1000°C, considering different electrochemical and thermal properties of the cell. The findings indicate that elevated operating temperatures facilitate electrochemical reactions, resulting in enhanced ionic conductivity and reaction kinetics, which ultimately improves the overall performance of the SOFC.

The second objective was to characterize the resulting current and power densities across varying temperature conditions. The objective was achieved through the analysis of the current-voltage (I-V) and power-voltage (P-V) characteristics derived from the simulations. The results indicated that increasing temperature led to enhancements in both current and power densities, with an optimal balance occurring at approximately 800°C. At excessively high temperatures, material degradation and thermal stress emerged as significant concerns.

The third objective aimed to validate the simulation model through a comparison of results with published experimental and literature data. A comprehensive comparative analysis demonstrated a strong correlation between the simulated and experimental data. The model achieved over 90% accuracy and 18.58% increment in current density at 800°C compared to Jawad Hussain's Model [35], thereby confirming its reliability and applicability in predicting SOFC behaviour across various operating conditions.

This research offers insights into optimizing SOFC performance through the management of operating temperatures, selection of suitable materials, and refinement of structural designs. The successful attainment of research objectives facilitates further progress in SOFC technology, promoting improved efficiency and durability.

5.2 Future Work

Future research on SOFCs should concentrate on several critical areas to improve the efficiency and durability of these energy systems. Refining the existing simulation model by incorporating complex multi-physics interactions, including degradation mechanisms and transient operating conditions, will yield a more accurate representation of real-world performance. Further investigation into advanced materials exhibiting enhanced thermal and electrochemical stability may result in improved long-term performance and decreased degradation rates.

Future research should focus on optimizing the geometric design of solid oxide fuel cell components to improve thermal management and reduce mechanical stress. This can be accomplished via topology optimization and sophisticated computational techniques to determine the most efficient configurations. The integration of hybrid energy systems, including the combination of SOFCs with renewable energy sources and energy storage solutions, warrants investigation to evaluate their feasibility and potential benefits.

Experimental validation of the enhanced simulation models via prototype testing is essential for confirming the reliability and applicability of the proposed optimization strategies. Collaborative research with industry partners can aid in transitioning theoretical findings to practical applications, promoting the commercial adoption of optimized SOFC systems.

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