MULTIPHYSICS MODELING, SIMULATION AND OPTIMIZATION OF SOLID OXIDE FUEL CELLS AND ELECTROLYZERS

A dissertation submitted
in partial fulfilment of the requirements for the award of degree of

Master of Engineering (M.E.)
in
CAD/CAM Engineering
by

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PATIALA
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I hereby declare that the dissertation entitled "**Multiphysics Modeling, Simulation and Optimization of Solid Oxide Fuel Cells and Electrolyzers**" is an authentic record of my work carried out in my internship at Bosch Global Software Technology (BGSW) and as a requirement for the award of the degree of Master of Engineering in CAD/CAM Engineering at Thapar Institute of Engineering and Technology, Patiala under the support and guidance of Dr. Vineet Srivastava (Associate Professor) and Dr. Kishore Khanna (Assistant Professor), Mechanical Engineering Department. I hereby declare that in case of violation of the intellectual property rights or copyrights found at any stage, I will be solely responsible for the same. And no part of the matter embodied in this report has been submitted to any other university or institute for the award of any degree.

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DECLARATION

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I further affirm that I have adhered to the ethical guidelines and principles of academic integrity throughout the research and compilation of this project.

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Aashish

Aashish

Dedicated to my family

For their endless love, support and encouragement

Abstract

This M.Tech Thesis explores the topic of solid oxide fuel cells (SOFCs) and Solid oxide electrolyzer cells (SOEC's) simulation using COMSOL Multiphysics, discussing the critical need for modeling and simulation tools in the development and optimization of these energy conversion devices. The thesis discusses the fundamental principles of SOFC's and SOEC's and the challenges associated with their design and performance. This report also highlights the advantages of simulation-based approaches in overcoming these challenges and enabling the exploration of various design and operational parameters.

Testing of fuel cells is a highly costly task and if we have to do it for multiple parameters, then it will take huge time to market and increase substantial cost for research and development and ultimately pass it on to the end user. Using simulation techniques which can capture and couple electrical part, chemical part and fluid dynamics part can help reducing that time, money and effort. The general methodology to model and simulate almost any type of fuel cell is well explained.

This study is intended to find and document the procedure to model Solid Oxide Fuel cell in COMSOL Multiphysics® using Electrochemistry module in COMSOL. Thereafter this study will certainly help in the understanding the basics of Cell level modeling and thus help in optimization of cell performance by studying the impact of various input parameters like pressure, temperature, Gas diffusion electrode porosity, Cell length and Electrode thickness.

A 3D model of an anode-supported planar reversible solid oxide cell (rSOC) will be developed in the future scope and is currently in the pipeline. The model incorporates multiple physical phenomena, including reversible electrochemistry and charge transport, as well as momentum, mass, and heat transport. Using a unit-cell level geometry, the model assesses the performance of the cell in terms of current-voltage (j-V) characteristics in both fuel cell and electrolysis modes.

Apart from this master thesis discusses the methodology for modeling any type of electrolyzer cell using Fuel cell and electrolyzer module in COMSOL Multiphysics.

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Nomenclature

Abbreviation	**Description**
SOFC	Solid oxide fuel cell
SOEC	Solid oxide electrolysis cell
MSR	Methane steam reforming
WGS	Water Gas Shift
B-V	Butler- Volmer
TPB	Triple phase boundary
GDE	Gas diffusion electrodes
GDL	Gas diffusion layer

Symbols

Symbol	**Description**
α	Charge transfer diffusion coefficient
ε	Porosity
η	Over potential in V
κ	Permeability
μ	Dynamic viscosity
F	Faraday’s Constant
V_{rev}	Reversible voltage (Theoretical)
V_{act_cath}	Activation loss at cathode
V_{act_anode}	Activation loss at anode
V_{ohmic}	Ohmic losses due to resistance
V_{conc_anode}	Concentration losses at anode
V_{conc_cath}	Concentration losses at cathode

Chapter 1

Introduction

1.1 Introduction

The increasing demand for energy resources is a growing and inevitable problem that the world is facing, caused in large part by the rising global population; projections show that world primary energy demand is expected to rise by 40% by 2030, with the global population projected to grow to 8.2 billion, particularly in Africa & Asis, which will experience the most rapid acceleration of growth, while the populations of Europe and Japan are expected to either slightly increase or fall. One way to tackle this problem is by shifting to greener and decentralized methods of Energy production. In this regard Fuel Cells role comes into picture.[1]

Fuel cells are machines that transfer energy from a gaseous or gasified fuel directly into electricity and heat through electrochemical reactions with an oxidant. One example is the high-temperature fuel cell known as SOFC. Fuel cells are considered environmentally friendly due to their high efficiency and low emission of pollutants during electricity production. Additionally, solid oxide fuel cells have gained significant attention lately due to their growing versatility in utilizing multiple fuel sources.[2]

This report focuses specifically on conducting three-dimensional simulations of Solid Oxide Fuel Cells (SOFCs) and Solid Oxide Electrolyzer Cells. The high operating temperature of SOFCs makes it challenging and expensive to experimentally investigate and measure various parameters associated with them. As a result, mathematical modeling plays a crucial role in evaluating the performance of SOFCs, as well as identifying and addressing the challenges encountered during their development.

Firstly, a basic approach is given for the electrochemical modeling of solid oxide fuel cell with electrochemistry module is given, then a parametric study is done to study the effects of individual input parameters on the performance of the fuel cell under various conditions and then combined effects of all parameters has been taken into account simultaneously

1.2 Basics of Fuel Cells

Fuel cells are efficient and environmentally-friendly devices that harness the chemical energy of hydrogen or other fuels to generate electricity. When hydrogen is used as the fuel, the only by-products produced are electricity, water, and heat. What sets fuel cells apart is their versatility in terms of potential applications. They can utilize a diverse range of fuels and feedstock's, enabling them to power a wide array of systems, from utility power stations to compact devices like laptop computers.[3]

1.2.1 Basics of Solid Oxide Fuel Cells

Within the solid oxide fuel cell, hydrogen and oxygen gas molecules undergo a process of dissociation, breaking down into their elemental components before reacting with each other. This reaction generates direct current (DC) electricity, which is then converted into alternating current (AC) through an inverter. Alongside the electricity generation, heat and water are also produced as by products. The heat can be utilized by transferring it to a heating system via an optional heat exchanger, providing heat energy for applications such as heating service water. The electrochemical reaction occurs within a temperature range of 500 to 700 degrees Celsius. One remarkable aspect of this power generation method is its minimal production of nitrogen oxide and particulate matter. Moreover, when pure hydrogen is used as the fuel, no carbon emissions occur, contributing to the fuel cell's sustainability advantages over other conventional power plants.[4]

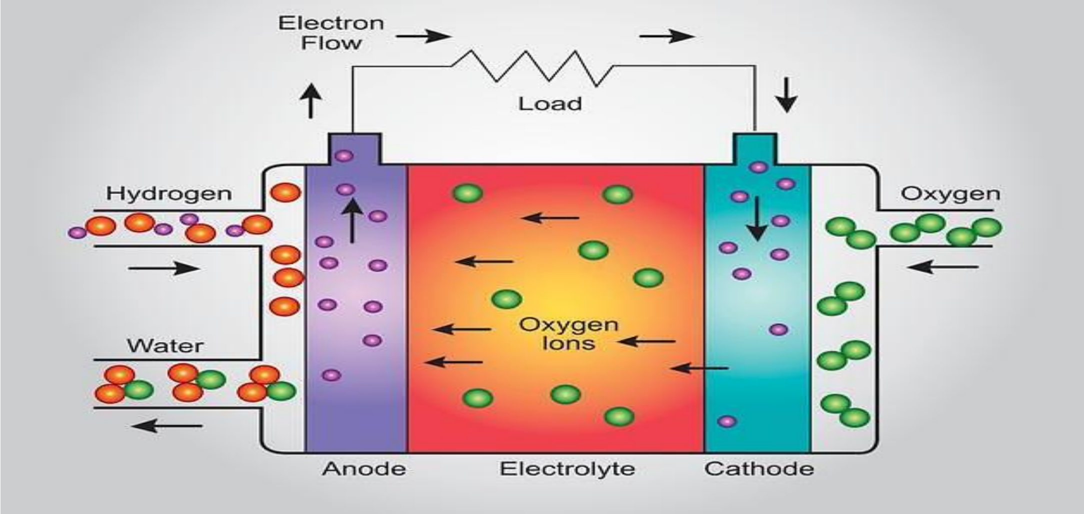


Figure 1: Solid oxide fuel cell [18]

1.2.2 Basics of Solid Oxide Electrolyzer Cell

A solid oxide electrolyzer cell (SOEC) is essentially a solid oxide fuel cell operating in regenerative mode. It facilitates the electrolysis of water (and/or carbon dioxide) by utilizing a solid oxide, or ceramic, electrolyte. This process results in the production of hydrogen gas (and/or carbon monoxide) and oxygen. The production of pure hydrogen holds great significance as it serves as a clean fuel that can be stored, positioning it as a potential alternative to batteries, methane, and other energy sources within the hydrogen economy.[17]

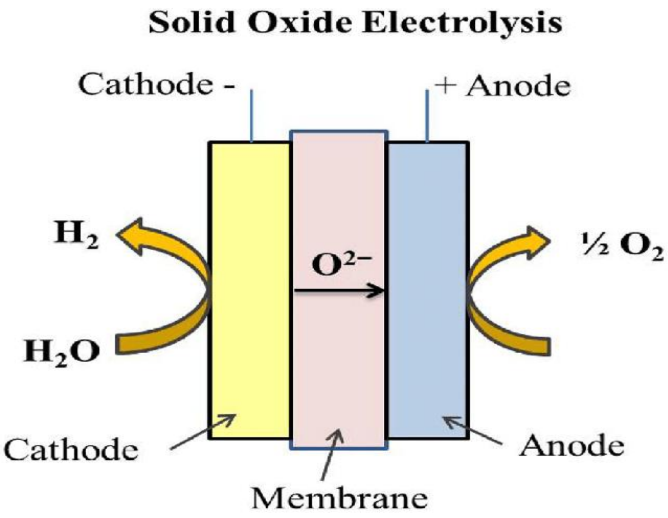


Figure 2: Solid oxide electrolysis process [19]

1.2.3 Chemical Reactions for SOFC

Power will be produced by SOFC

Inside Cell

- Anode: $H_2 + O^{2-} \rightarrow H_2O + 2^{e-}$
- Cathode: $0.5\ O_2 + 2^{e-} \rightarrow O^{2-}$
- Overall cell reaction: $H_2 + 0.5\ O_2 \rightarrow H_2O$ [6]

In Steam Reformer (if we use methane as input fuel)

- $CH_4 + H_2O$ (+ heat) → $CO + 3H_2$
- $CO + H_2O \rightarrow CO_2 + H_2$ (+ amount of heat)

1.2.4 Chemical Reactions for SOEC

Power will be consumed by SOEC

- Cathode: $H_2O+2^{e-} \rightarrow H_2 + O^{2-}$
- Anode: $O^{2-} \rightarrow ½\ O_2 + 2^{e-}$
- Overall cell reaction: $H_2O \rightarrow H_2 + ½\ O_2$

1.2.5 Fuel Cell Structure

Anode, electrolyte, and cathode are the three basic components of a single fuel cell. The anode and cathode sides are each given a fuel and an oxidant that are provided by outside sources. Any gas that can be electrochemically oxidised and reduced could be used for both. The driving force behind the process is the chemical potential gradient of ions across the electrolyte. As a result, the external circuit produced direct-current power. To enhance the overall outlet voltage in practical applications, fuel cells are connected in a series configuration. To establish an electronic connection between the cathode of one cell and the anode of the next cell, an interconnect plate is always installed.[20]

1.2.5.1 Electrolyte

For a material to be suitable as an electrolyte in fuel cells, it must possess specific properties. These requirements are crucial to achieve optimum cell performance. Some of the key properties that oxide electrolyte materials must meet include:

- High oxide ion conductivity (or proton conductivity) within a specific thickness range (0.01-0.1 S cm-1)
- A low electronic conductivity is necessary to prevent the generation of electricity within the electrolyte.
- Chemical stability: The electrolyte material must be chemically stable under conditions of oxygen potential gradient

1.2.5.2 Electrode

There are generally two main electrodes in a fuel cell as well as electrolyzer cell, one is Cathode Gas diffusion electrode and anode gas diffusion electrode [1]

- **Catalytic activity:** Electrodes in fuel cells must have high catalytic activity to promote the chemical reactions that occur at the electrodes. For example, the anode in a hydrogen fuel cell must catalyze the oxidation of hydrogen to form protons and electrons.
- **High Electrical conductivity:** Electrodes in fuel cells must be good electrical conductors to allow the transfer of electrons between the electrode and the external circuit.
- **Porosity:** Electrodes must be porous to allow for the flow of reactants and products to and from the electrode surface. This facilitates efficient reaction rates and prevents build-up of reaction products that can interfere with the reaction.
- **Stability:** Electrodes must be stable under the conditions of the fuel cell environment. They must not corrode or degrade over time, which could result in reduced efficiency or complete failure of the fuel cell.
- **Surface area:** The surface area of the electrodes is important for increasing the number of

reaction sites and promoting efficient reaction rates. Therefore, electrodes in fuel cells are typically designed to have a high surface area per unit volume.

- **Compatibility:** Electrodes in fuel cells must be compatible with the fuel cell electrolyte and other materials used in the fuel cell to prevent degradation of the fuel cell components and to promote efficient operation

1.2.5.2.1 Cathode Gas diffusion electrode (SOFC)

In a fuel cell operating in an oxidizing environment of air or oxygen at high temperatures, the cathode air electrode plays a critical role in the oxygen reduction reaction. Some key aspects of the cathode air electrode's function in this environment are:

- Stability of chemicals and dimensions in the oxidising environment that cells operate in
- Compatibility with the other cell components in terms of thermal expansion
- The electrolyte and the connector that the air electrode comes into touch with must be compatible and have a low amount of reactivity
- Enough porosity to make it easier for molecular oxygen to be transported from the gas phase to the air electrode/electrolyte interface.

1.2.5.2.2 Anode Gas diffusion electrode (SOFC)

The anode gas diffusion electrode in a fuel cell is responsible for facilitating the oxidation of hydrogen and oxygen ions, resulting in the production of water and excess electrons, which then pass through the electrical circuit to generate electricity. To perform this role effectively, the anode gas diffusion electrode should possess the following properties:

- High electronic conductivity
- Stability in a reducing environment
- Thermal expansion properties matching other cell components
- Compatibility and minimal reactivity
- Sufficient porosity

1.2.5.3 Interconnects

The interconnect material needs to maintain stability when exposed to both oxidizing and reducing atmospheres since it comes into contact with both electrodes. Additionally, it should possess electronic conductivity and exhibit characteristics similar to those of the electrolyte. Apart from ensuring chemical compatibility, it is crucial for the coefficient of thermal expansion to be co-aligned with different components of the cell to prevent stress formation under operational conditions. Among all the components of the cell, the interconnects face the most stringent requirements due to their exposure to both fuel and air atmospheres. [21].

- They should exhibit almost 100% electronic conductivity.
- The stability of the electrolyte material is essential in both oxidizing and reducing atmospheres at the operating temperature of the fuel cell.
- To prevent direct combination of oxidant and fuel during cell operation in planar designs, they should have low permeability to oxygen and hydrogen. Their thermal expansion coefficient should be similar to that of the other materials used in the cell to avoid the generation of stress.
- They should not react with other materials in the cell.

1.2.5.4 Sealants

The sealants must satisfy all requirements for each component. They must be capable of operating safely at high temperatures while remaining stable in a wide variety of oxygen partial pressures (air and fuel). High-quality seals are essential because even tiny leaks in them can damage the cell potential and lower performance. Because the ideal sealant depends on the materials of other components, sealant development is more difficult.[21]

1.2.6 Fuel Cell Operating Principle

Fuel cells operate based on the principle of an oxygen-ion conducting electrolyte, where oxide ions move from the cathode side to the anode side. The fuel is directed through the fuel channel and flows into the anode region until it reaches the interface between the anode and electrolyte. At this interface, the fuel undergoes oxidation, releasing electrons into the electronically-conductive anode. These electrons are then directed towards the interconnects and subsequently flow through the external electric circuit. [22]

1.2.7 Main Components for SOFC system

Fuel Reformer – To convert methane into hydrogen before going into the stack, also separating other gases produced thereby during WGS and SR reactions

Heat Exchangers – To recover waste heat on various places thereby improving overall efficiency

Burners – To recover chemical energy from leftover fuel coming out of the stack and also to heat stack to initial temperature (to begin reaction)

Fuel Cell Stack – The main heart of the system (where magic happens)

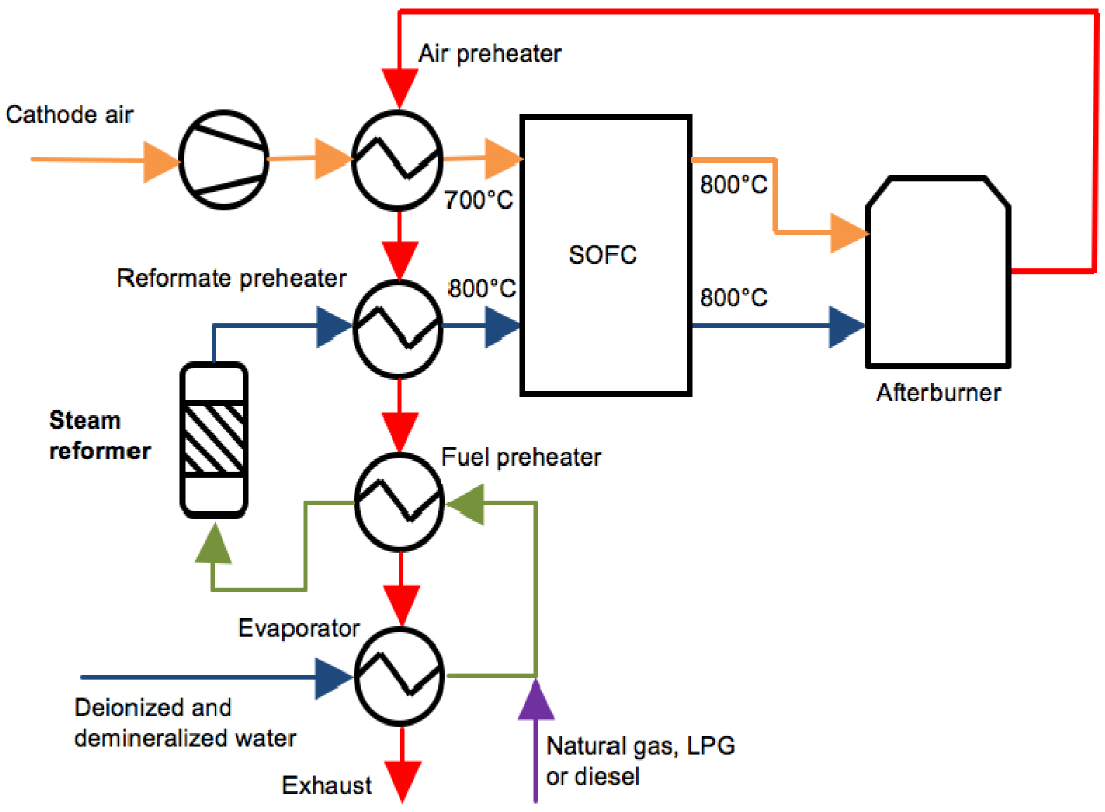


Figure 3: Auxiliary components used with SOFC (Not a standard design)[7]

1.2.8 Types of Fuel Cell Designs

There are basically 2 main types of designs for fuel cells (mainly for SOFC)

Planar and Tubular designs

- Tubular design is mostly used where cost is of prime importance and planar is used where power density is of prime importance.
- One of the design offers high power density and another one offers better sealing capabilities in the cell level.
- There are also some other types of designs that are available but they are currently in development phase only and are not being used commercially.

a. Planar Design

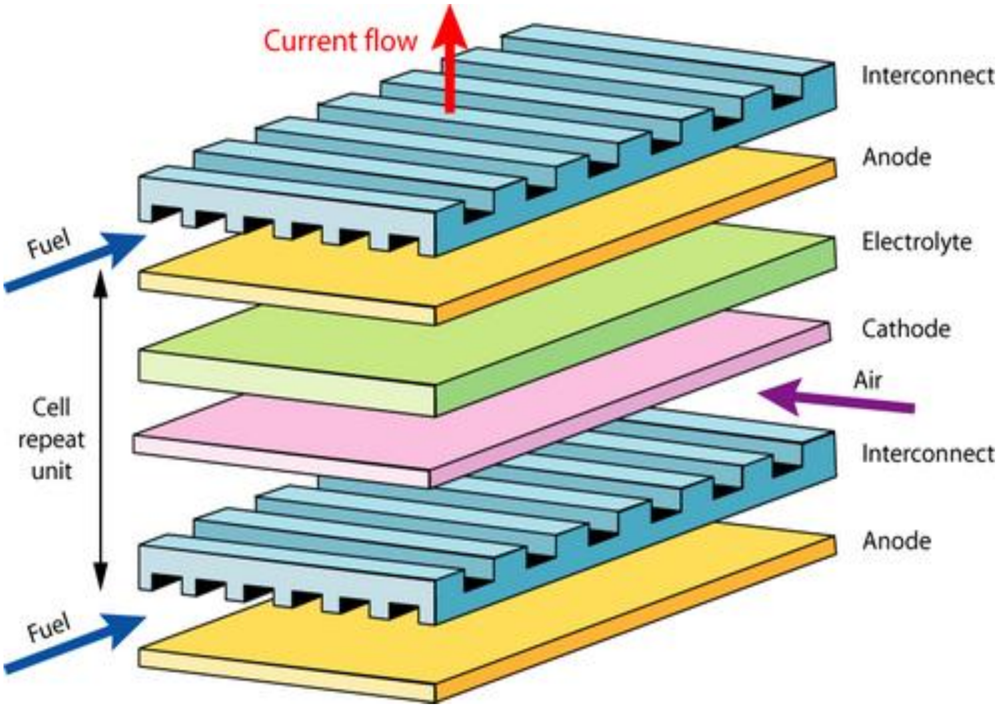


Figure 4: Planar fuel cell design [23]

Planar Fuel Cells are composed of flat layers stacked vertically. This design enables the construction of Fuel Cell stacks by simply stacking multiple Fuel Cells on top of each other, resulting in a straightforward and high-power-density (W cm^{-3}) configuration. However, there are several notable drawbacks associated with the planar design:

- Gas-tight sealing is required around the edges of the cell components, which adds complexity to the design and manufacturing process.
- Planar Fuel Cells tend to be brittle and susceptible to mechanical and thermal stress, which can compromise their durability and performance.
- Thin planar layers have limited scalability, making it challenging to increase the size and capacity of the Fuel Cell system.

b. Tubular Design

Tubular cells are comprised of three cylindrical layers arranged concentrically: the anode, electrolyte, and cathode materials. When multiple tubular Fuel Cells are combined, they form a stack composed of a bundle of Fuel Cell tubes.

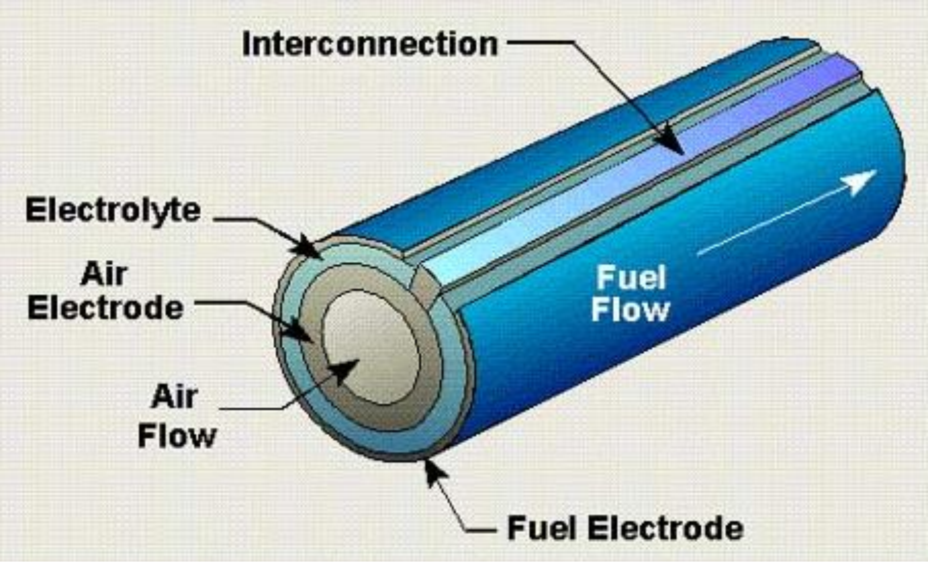


Figure 5: Tubular SOFC design [24]

The tubular design effectively addresses the brittleness and sealing challenges encountered in planar cells. However, this geometry comes with certain drawbacks, including higher fabrication costs and lower power densities. These limitations arise from the lengthy path that electrical power must traverse within each cell and the presence of significant voids within the stack structure.

1.2.9 Barriers for SOFC

There are basically two types of the most important barriers in the development of solid oxide fuel cells as well as Electrolyzers.

1.2.9.1 Technical Barriers for SOFC[7a]

- High Startup time due to very high initial temperature required (usually 500 to 1000 degree Celsius)
- System design life (components life degradation)
- Inadequate stack durability
- Lack of robustness and insufficient reliability of stacks
- High temperature corrosion and breakdown of cell components

1.2.9.2 Economic Barriers for SOFC

- High initial investment
- High LCOE (Levelized cost of Energy)
- High cost of stack replacement (re-investment for customer)

- Limited availability of financing models to overcome cost hurdle

1.2.10 How do we measure performance of a Fuel Cell ?

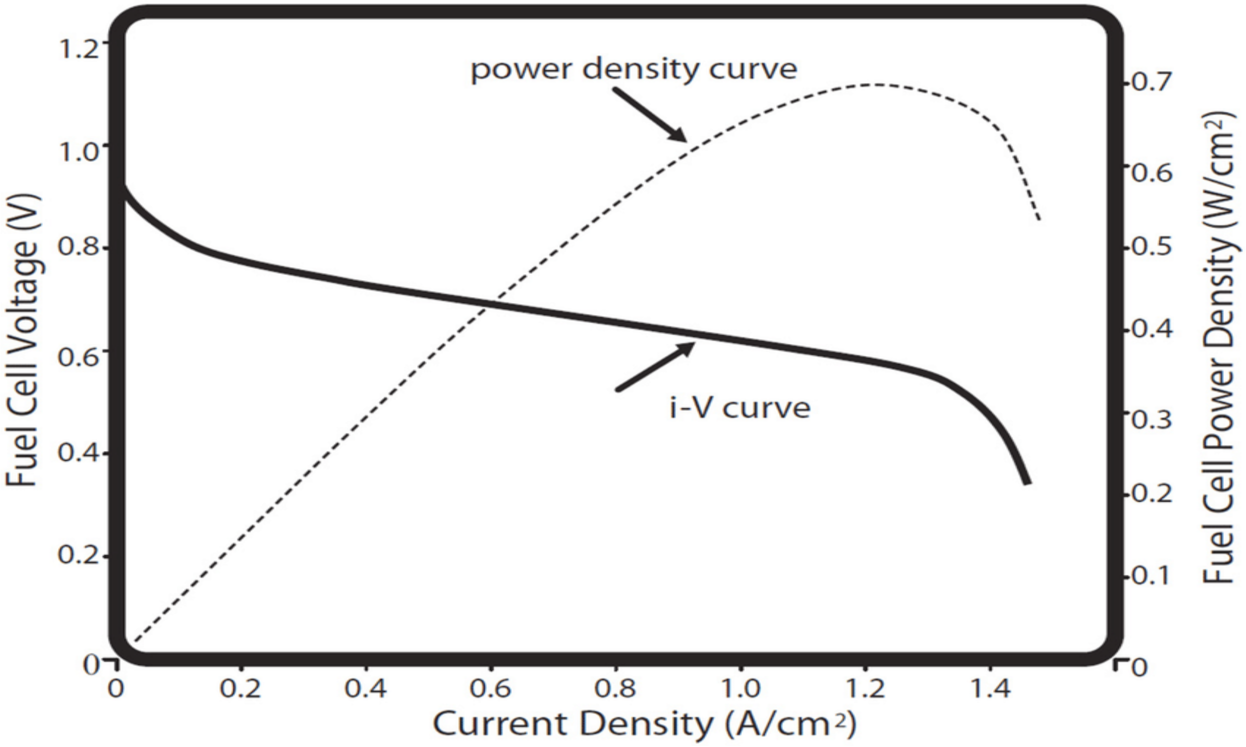


Figure 6 – Polarization curve [8]

1.2.10.1 Basics of Polarization Curve

- Polarization curve is the most fundamental and standard in situ diagnostic technique for assessing the performance of SOFC [9]
- In testing it is usually obtained with a potentiostat/galvanostat
- Power vs Density curves are also used alongside polarization curve

1.2.11 Safety Precautions

The overall safety strategy for handling fuel cell systems should be developed based on the following sequence

- Ensure measures are in place to prevent the accidental release of combustible, toxic, and pollutant gases, liquids, and solids.
- Implement suitable safety markings to effectively communicate the remaining risks and hazards.[25]

CHAPTER 2

Literature Review

A survey of available literature suggests that **Zhao et al. 2004** [26] studied the dependence of various cell parameters like electrolyte thickness, temperature, porosity and anode electrode thickness on polarization curves via experimental testing and concluded that with increasing temperature, the power density was increasing and the same effect was noted with the average current density. His team also studied the effect of reducing the electrolyte thickness on polarization and power density curves.

Gerasimov et al.[27] from Ansys tried to simulate the tubular SOFC 3D model using user defined functions in Fluent software. Their model used anode inlet of 2.5×10^{-7} Kg/sec of humidified hydrogen at 973 K. Then they analyzed the polarization curves, temperature distributions on anode, cathode and electrolyte interfaces. They also analyzed Nernst potential, current density distributions and voltage distributions throughout the length of the cell. Apart from this they analyzed mole fractions of all species like H_2, H_2O, O_2, N_2 etc.

Hesami et al. 2021 [28] investigated the effect of interconnect design on the performance of planar SOFC using COMSOL Multiphysics and compared with experimental results data and found that this simulation technique is at par and sufficient to capture the Multiphysics with just a 6% deviation with experimental data and that too at the highest mark, (at some locations the error was less than 1 %).His team also analyzed the channel shapes like rectangular, triangular and trapezoidal on the performance aspect of SOFC

Peksen et al. 2010 [29] investigated the 3D Multiphysics Modeling in the Design and Optimization of SOFC System Components. They compared the predictions of simulation data for preheater and compared with test data at Research Centre Jülich SOFC components. A comprehensive multiphysics analysis, incorporating fluid flow, heat transfer, chemically reacting species transport, and thermo mechanics of the integrated module components, has been suggested. The results of stand-alone analyses were found to be reasonable, effectively capturing the behavior of individual components and providing valuable insights.

Sleiti et al. 2010 [30] In their study, the researchers examined how temperature and cathode porosity impact the performance of a Solid Oxide Fuel Cell (SOFC) system. To capture the complex multiphysics phenomena in the SOFC system, they utilized ANSYS Fluent software and implemented user-defined functions. The researchers conducted a parametric study, varying the temperature from 500 to 700 degrees Celsius and adjusting the cathode electrode porosity from 10% to 30%. Through their analysis, they observed that decreasing the porosity of the Cathode Gas Diffusion Layer (GDE) led to an increase in voltage. Based on their findings, the researchers concluded that SOFC systems can achieve higher efficiency in intermediate temperature ranges when operating under low porosity conditions, assuming other parameters remain constant.

Liu at al. 2002 [31] investigated the experimental validations on Anode supported SOFC working on Methane and Natural Gas .They tested two cells basically i.e. LSM-YSZ and LSCF-GDC and concluded that the cell shows a good stability with methane and natural gas when operated for more than 90 hrs. with methane. Finally, they concluded that results show that conventional anode supported SOFCs can be operated directly with humidified methane and natural gas, yielding high open circuit voltages and high power densities.

Blum et al. 2012 [32] Forschungszentrum Jülich GmbH SOFC team investigated 450 different types of fuel cells ranging between 100 W to 15 kW.In their experimental testing long term stability has improved in a way that in a test lasting more than 11,000 hours, a degradation rate below the target for stationary operation is achieved. They constantly monitored the performance during this prolonged testing and found out that with metal interconnects there is no such drop in power density and current density which ultimately denotes the performance aspects of the cell.

Peksen et al. 2009 [33] The researchers conducted a study in which they developed and experimentally validated a computational fluid dynamics (CFD) model of a Julich type pre-reformer. They employed a continuum modeling approach and successfully demonstrated its feasibility. The model accurately represented the design of the pre-reformer and the properties of its various components, including the air channels, solid frame, wire mesh structures, and catalyst. Parameters such as permeability, porosity, mass flow rate, temperatures of air and fuel gas, and chemical reaction data were determined through experimental measurements conducted in Julich. The researchers proposed that the developed model could serve as a cost-effective tool for optimizing the processes taking place within the pre-reformer, replacing the need for expensive and impractical experiments.

Celik et al. 2018 [34] proposed a three-dimensional model of a planar SOFC using CFD approach. They proposed the most detailed study available till date to provide all the operational parameters. They coupled the thermal , electrical and chemical approach. They used COMSOL Multiphysics software to completely capture the multi-dimensional and Multiphysics approach of the problem. They, then validated the simulation results with the experimental validation. The molar fraction of the gas mixture that they used is 80% H_2 and 20 % water at the anode side. On the cathode side, they used the air only instead of pure oxygen. Then they varied hydrogen and oxygen molar fractions and analyzed the impact on the performance of SOFC unit

2.1 Analysis of Literature Review

- Most of the papers have considered the experimental testing of SOFC and its components because at that time, capturing all physics and chemistry simultaneously was very challenging part. (simply because computational cost were very high and simulations were not accepted as mainstream).Experimental testing was a time consuming process overall as compared to simulations and a very expensive one too.
- Some papers considered CFD approach but there methods were limited because they have to write user defined functions inside software’s which makes research scope limited to constant variables
- Many parameters cannot be captured using experiments like species distribution inside the cell, current density variation etc.

2.2 Research Gap

- Most of the previous research is focused on Ansys Fluent software which inherently assumes the electrolyte as a solid wall with porosity and thereby neglecting other properties like its ionic and electrical conductivity which will be temperature dependent, thereby reducing accuracy of solution.
- Some papers have just considered one or two operational parameters in their study and a detailed parametric study considering multiple parameters was missing in these papers.
- Most papers considered pure oxygen in SOFC cathode side, which is impractical as the testing that they have referred to uses air which will have Nitrogen, oxygen and other gases as well which will decrease the rate of chemical reaction.
- There is no paper till now (as per my understanding) which considers both SOFC and SOEC with detailed methodology approach of modeling both of them with all assumptions and software limitations.

CHAPTER 3

Design of a 15 kW SOFC System

This section deals with the calculation of a Solid oxide fuel cell system regarding mass flow rates of hydrogen, methane oxygen and nitrogen calculations for a 15 kW SOFC system.

After oxygen calculation, we will estimate the amount of pure air that needs to be supplied for the same power output, considering some factor of safety as well.

3.1 Assumptions used

- Average Operating Temperature is 650 ℃
- Considering pure Hydrogen going into SOFC Stack
- Assuming 1 Cell Voltage as 0.7 $Volts$ after Polarization Losses
- Assuming 80 % Fuel Utilization Factor in SOFC
- Air requirement is 4 times the required one
- Efficiency of reformer is 80 %
- Considering 1.5 Mole of Water requirement per 1 Mole of CH_4

3.2 Hydrogen mass flow rate required from Power output

- Gas Constant R for $\mathrm{CH_4} = 518.28\ {}^{\mathrm{J}}/_{\mathrm{kgK}}$
- $\mathrm{R\ for\ O_2} = 259.84\ {}^{\mathrm{J}}/_{\mathrm{kgK}}$
- $\mathrm{R\ for\ H_2} = 4124.2\ {}^{\mathrm{J}}/_{\mathrm{kgK}}$
- $\mathrm{Faraday's\ constant} = 96485.3321\ {}^{\mathrm{C}}/_{\mathrm{mol}}$

  $\mathrm{Power\ required} = \mathrm{Voltage}\ \times \mathrm{Current}$

- $1500\ \mathrm{Watts} = 0.7\ \mathrm{Volt} \times \mathrm{I\ ampere}$
- $\mathrm{Current} = {}^{15000}/_{0.7} = 21428.571$
- $\mathrm{H_2}$ required (mole / second) Current/ (number of free electrons × Faraday's Constant)
- $\mathrm{Hydrogen\ Required}\ = {}^{\mathrm{I}}/_{\mathrm{nF}} = \frac{21428.571}{2 \times 96485.3321} = 0.111\ \mathrm{mole\ /second}$

- To convert it into $\frac{\text{gm}}{\text{second}}$, we have to multiply with its Molecular weight in $^{\text{gm}}/_{\text{mol}}$
- Hydrogen required (in gm/sec) $= 0.111 \times 2.016 = 0.2237\ ^{\text{gm}}/_{\text{sec}}$
- Hydrogen Supplied $= {}^{\text{Hydrogen Consumed}}/_{\text{Fuel Utilization Factor}}$
- Hydrogen supplied $= {}^{0.2237}/_{0.8} = 0.2796\ ^{\text{gm}}/_{\text{sec}}$

3.3 Calculation of Methane Consumption

From Mass Balance

- $CH_4 + H_2O = CO + 3H_2$
- $CO + H_2O = CO_2 + H_2$

From Above Reaction, we have 4 $Moles\ of\ H_2 = 1\ Mole\ of\ CH_4$

- 4×2.016 gm of $H_2 = 16 \times 0.2796$ of CH_4
- CH_4 consumed $= 0.5547\ ^{\text{gm}}/_{\text{sec}}$ for 15 kW design
- In kg/$_{\text{sec}}$ consumption is 5.547×10^{-4}

3.4 Calculation for Oxygen requirement

Reaction at ANODE

- $H_2 + O^{2-} = H_2O + 2^{e-}$

Reaction at Cathode

- $0.5\ O_2 + 2^{e-} = O^{2-}$

From Above, 1 Mole of H_2 requires 0.5 Mole of O_2

- 1×2.016 gm of $H_2 = 0.5 \times 32$ gm of O_2
- $1 \times 2.016 \times 0.2796$ of $H_2 = 0.5 \times 32$ of $O_2 = 16 / 0.5636 = 28.38$ gm/ sec of Pure O_2
- Air Calculation from $O_2 = 21\%$ of Air $= 28.28$ gm of O_2

- 100 % of Air $= (^{28.28}/_{21}) \times 100$
- Air will be 135.142 $^{\text{gm}}/_{\text{sec}}$ as per stoichiometry

3.5 Actual amount of Air supplied to stack

- For the safe side we will supply about 3 to 4 times more Air than requirement
- Actual Air supplied $= 4 \times$ Stoichiometric Requirement $= 4 \times 135.142 = 540.5714$ $^{\text{gm}}/_{\text{sec}}$ of Air

3.6 Extent of Reaction Calculation

The 2 main reactions happening in reformer when we are using methane are steam reforming reaction and water gas shift reaction

- $CH_4 + H_2O = CO + 3H_2$
- $CO + H_2O = CO_2 + H_2$

Considering 80 % efficiency of Reformer

- Reformer Efficiency $= (CH_{4_{in}} - CH_{4_{out}}) / CH_4$
- Assuming 1 Mole of CH_4 going in $0.8 = (1 - CH_{4_{out}}) / 1$

  $CH_{4_{out}} = 0.2$ Mole
- Formula = In – Consumed + Generated = Out
- For $CH_4 = CH_{4_{in}} -$ extent $= CH_{4_{out}}$

  $= 1 - e1 = 0.2$ So, $e1 = 0.8$
- For H_20 considering 1.5 mole going (to be on the safe side)

  $$= 1.5 - e_1 - e_2 = n_2$$
  $$= 1.5 - 0.8 - e_2 = n_2$$
- For Carbon — Monoxide

  $$0 \text{ moles in } + e_1 - e_2 = n_3$$
- For Carbon — Dioxide

  $$0 \text{ moles in } + e_2 = n_4$$
  $$e_2 = n_4$$

- For Hydrogen Gas

$$0 \text{ moles in } + 3\,e_1 + e_2 = n_5$$
$$= 3e_1 + e_2 = n_5$$

- Considering Selectivity of CO / C O2 as 3 [35]

$$\text{So}, n_3/n_4 = 3$$
$$= (e_1 - e_2) / e_2 = 3$$
$$= (0.8 - e_2) / e_2 = 3$$
$$\text{So}, e_2 = 0.2$$

- Putting the values ofe_1 and e_2 in previous equations we get,

$$\text{CO moles out} = 0.6$$
$$\text{CO}_2 \text{ moles out} = 0.2$$
$$\text{H}_2 \text{ moles out} = 2.6$$
$$CH_4 \text{ moles out} = 0.2$$
$$\text{H}_2\text{O moles out} = 0.5$$

CHAPTER 4

Tubular SOFC simulation in ANSYS Fluent

4.1 ANSYS Fluent SOFC (beta) module capabilities

The desired features for a computational model for Solid Oxide Fuel Cells (SOFCs) include:

- Capability to simultaneously account for electric field, mass transport, species transport, energy transport, and electrochemistry phenomena.
- Effective solution of the electric field within all components of the cell, including both porous and solid regions, while considering ohmic heating in the bulk materials.
- Ability to handle and integrate electrochemical processes within the model. - Incorporation of tortuosity effects in porous regions to accurately represent the transport properties.
- Flexibility to simulate an arbitrary number of electrochemical cells arranged in a stack configuration.
- Capability to model high-temperature electrolysis processes.[36]

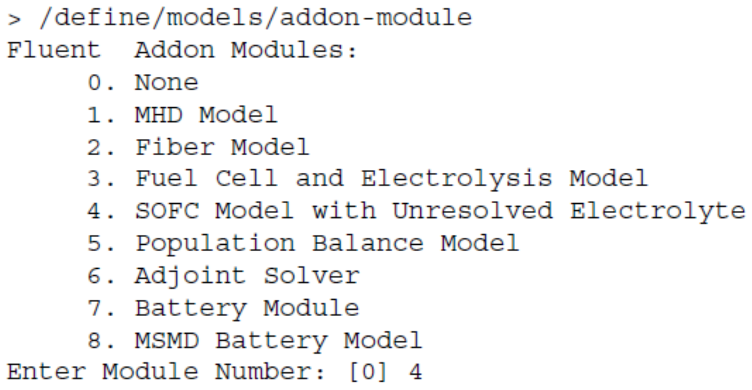
4.2 Assumptions used

- Anode exchange current density was assumed to be 1e+20 Ampere
- Cathode exchange current density was assumed to be 1000 Ampere
- Surface-to-surface radiation between internal boundaries is neglected
- Model considers electronic conduction between electrodes
- Electrochemical reactions happening at the triple phase boundary only
- Only Ionic conduction in the electrolyte and no electrical conduction
- Mass transport happening in porous electrodes
- Mole fraction reference values for H_2, H_20 and O_2 is taken as 0.8 , 0.2 , 0.21
- Anode and cathode Transfer coefficient as 0.5
- Viscous resistance value of 10^{13}litres per m^2
- Porosity of gas diffusion electrodes taken as 0.3
- Electrolyte resistivity of 0.2 ohm-m was considered for this study
- Current under relaxation factor of 0.4 was taken[36]
- Electrolyte resistivity of 0.2 $W/_m$was taken

4.3 Methodology

- The Solid Oxide Fuel Cell (SOFC) With Unresolved Electrolyte Model is loaded into ANSYS Fluent through the text user interface (TUI). It can be loaded from the following commands om the interface

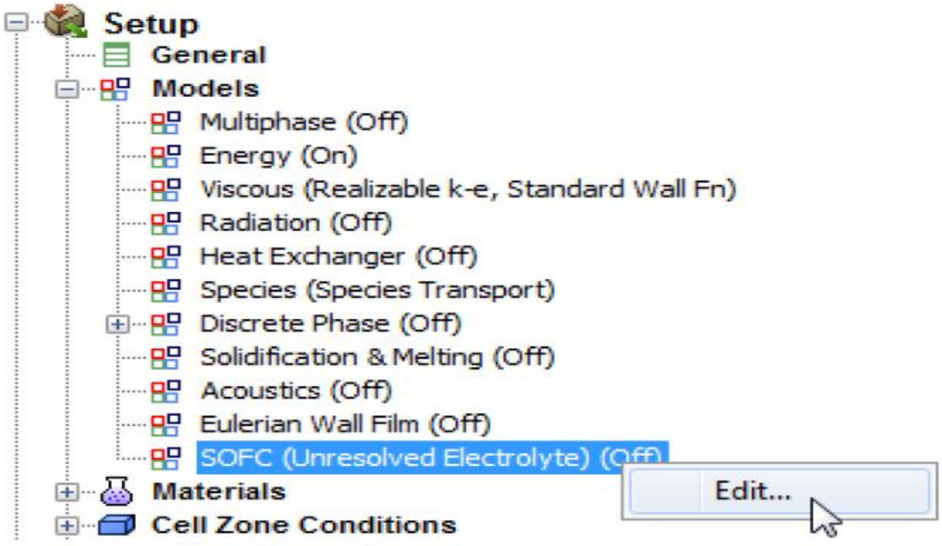
- define → models → add-on-module



```
> /define/models/addon-module
Fluent  Addon Modules:
        0. None
        1. MHD Model
        2. Fiber Model
        3. Fuel Cell and Electrolysis Model
        4. SOFC Model with Unresolved Electrolyte
        5. Population Balance Model
        6. Adjoint Solver
        7. Battery Module
        8. MSMD Battery Model
Enter Module Number: [0] 4
```

Figure 7 : [Screenshot] Advanced add-on modules ANSYS fluent

- After loading the module, the SOFC Model (Unresolved Electrolyte) option will become visible in the tree structure under the Models branch and can also be accessed in the Models task page.



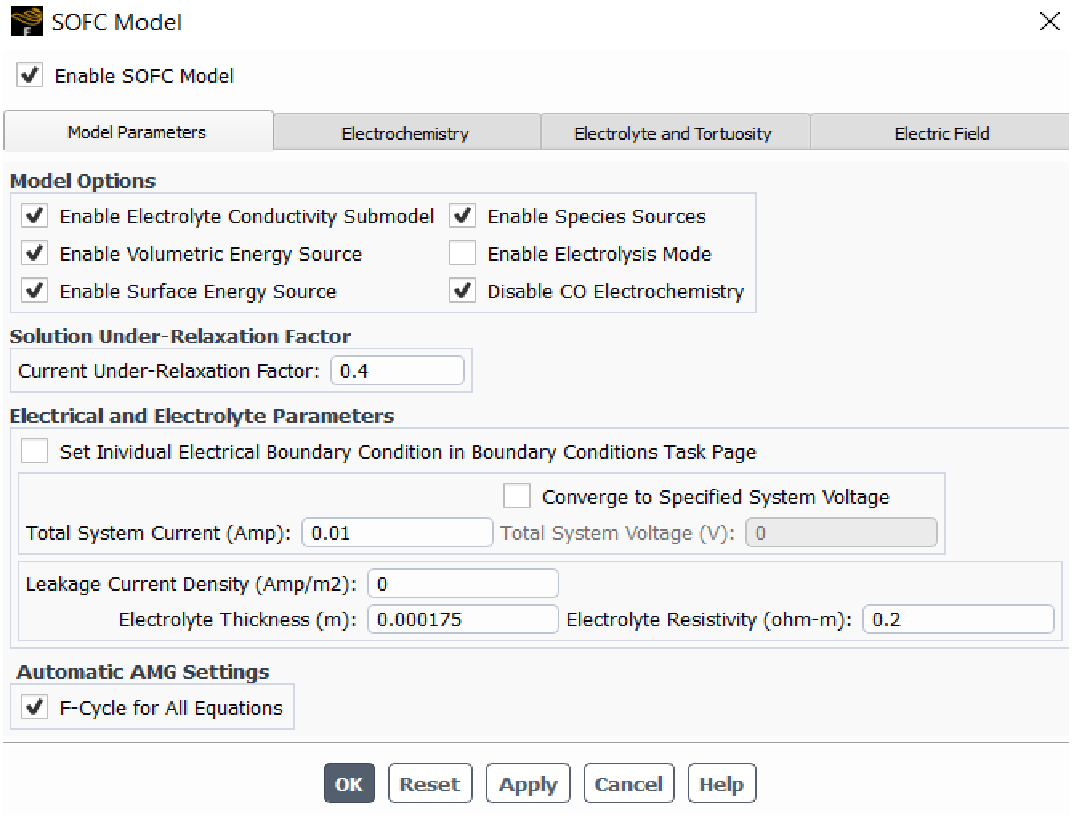
Setup
  General
  Models
    Multiphase (Off)
    Energy (On)
    Viscous (Realizable k-e, Standard Wall Fn)
    Radiation (Off)
    Heat Exchanger (Off)
    Species (Species Transport)
    Discrete Phase (Off)
    Solidification & Melting (Off)
    Acoustics (Off)
    Eulerian Wall Film (Off)
    SOFC (Unresolved Electrolyte) (Off)
  Materials
  Cell Zone Conditions

Figure 8 : SOFC module option after TUI selection

- Define various model parameters for the simulation
- In the **Species Model** dialog box, configure the following settings:

Setup → Models → Species Edit...

- Specify Electrochemistry parameters in the SOFC add on tab model
- Specify electrode and tortuosity parameters



☑ Enable SOFC Model

Model Options

☑ Enable Electrolyte Conductivity Submodel
☑ Enable Species Sources
☑ Enable Volumetric Energy Source
☐ Enable Electrolysis Mode
☑ Enable Surface Energy Source
☑ Disable CO Electrochemistry

Solution Under-Relaxation Factor

Current Under-Relaxation Factor: 0.4

Electrical and Electrolyte Parameters

☐ Set Inividual Electrical Boundary Condition in Boundary Conditions Task Page
☐ Converge to Specified System Voltage
Total System Current (Amp): 0.01
Total System Voltage (V): 0
Leakage Current Density (Amp/m2): 0
Electrolyte Thickness (m): 0.000175
Electrolyte Resistivity (ohm-m): 0.2

Automatic AMG Settings

☑ F-Cycle for All Equations

Figure 9: Model parameters in SOFC module

- Specify Electric field parameters for the current study
- Define material properties
- Set operating conditions: Specify temperature, pressure, and fuel/air flow rates.
- Define boundary conditions: Specify composition, temperature, and other parameters at various boundaries.
- Define convergence criteria: Set thresholds for solution convergence.
- Initialize the flow field: Provide initial values for variables such as velocity and species concentrations.
- Run the solution and post-process results: analyze and visualize the results using post-processing tools available in the software.

4.4 Model Description and Boundary conditions

In the SOFC system

- The anode inlet receives humidified hydrogen at a rate of $2.5 \times 10^{-7}\ {kg}/_{sec}$ and a temperature of 973 K.
- The cathode inlet is supplied with air at of $1.37 \times 10^{-5}\ {kg}/_{sec}$ and a temperature of 973K.

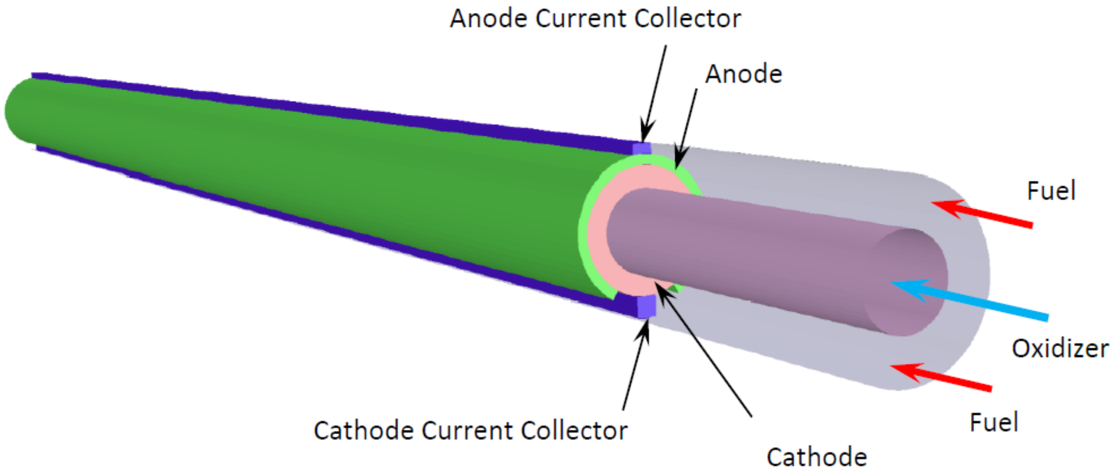
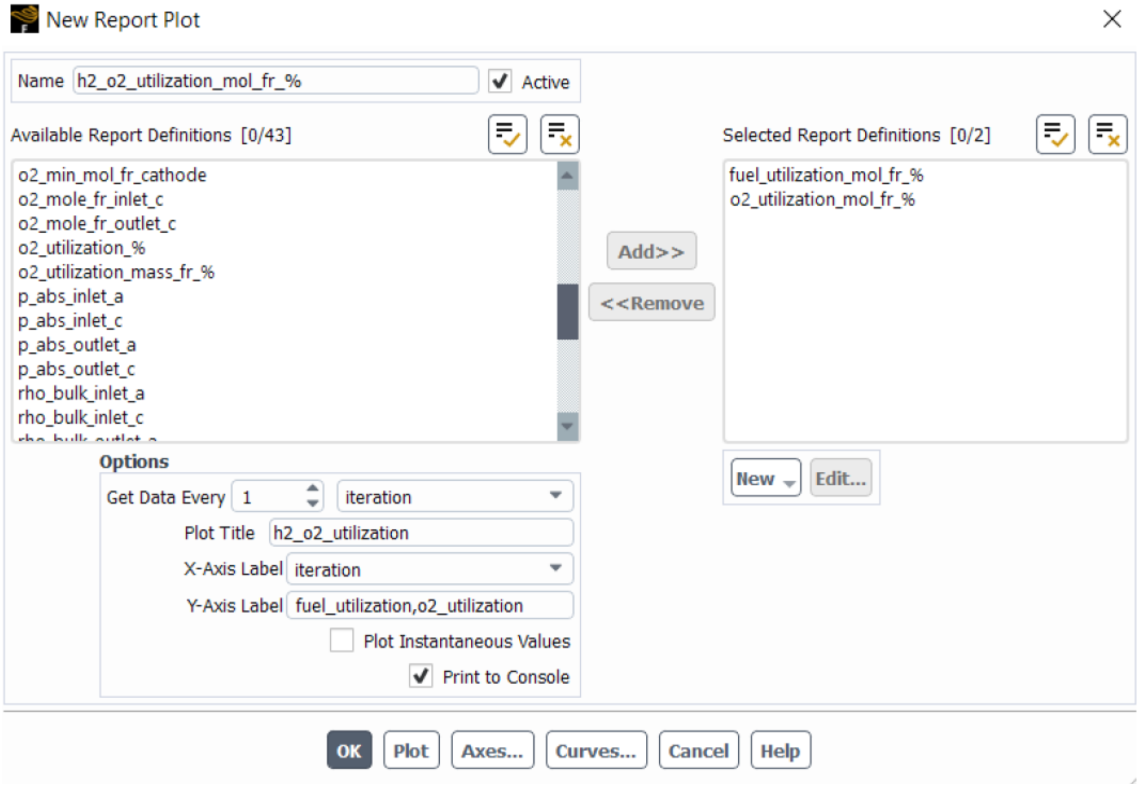


Figure 10: Tubular SOFC model [courtesy-ANSYS]

- Both the anode and cathode consist of two concentric cylinders, each with a length of 130 mm.
- The inner diameter of the cathode is 4 mm, while the outer diameter is 6 mm.
- The anode has an inner diameter of 6 mm and an outer diameter of 7 mm.
- The active electrolyte material, with a thickness of 20 microns, is pressed between the anode and cathode layers.
- The outer walls of the anode and cathode current collectors are adiabatic in this simulation.
- Fuel flows through the porous anode, while air flows through the porous cathode towards the electrolyte region.
- Electrochemical oxidation of fuel occurs at the interface between the electrolyte region and the anode.
- Electrochemical reduction of oxygen from incoming air takes place at the interface between the electrolyte region and the cathode.
- The overall reaction results in the formation of water on the anode side.
- Mass fractions for water and hydrogen are taken 0.52 and 0.48 respectively in the Species Mass Fractions group box
- setting up the report monitors in fluent is a challenging and time-consuming task and it has to be done every time we run the simulation, so it’s better to save a .tsv file to do such repetitive tasks once we save it



New Report Plot

Name h2_o2_utilization_mol_fr_% ☑ Active

Available Report Definitions [0/43]

o2_min_mol_fr_cathode
o2_mole_fr_inlet_c
o2_mole_fr_outlet_c
o2_utilization_%
o2_utilization_mass_fr_%
p_abs_inlet_a
p_abs_inlet_c
p_abs_outlet_a
p_abs_outlet_c
rho_bulk_inlet_a
rho_bulk_inlet_c

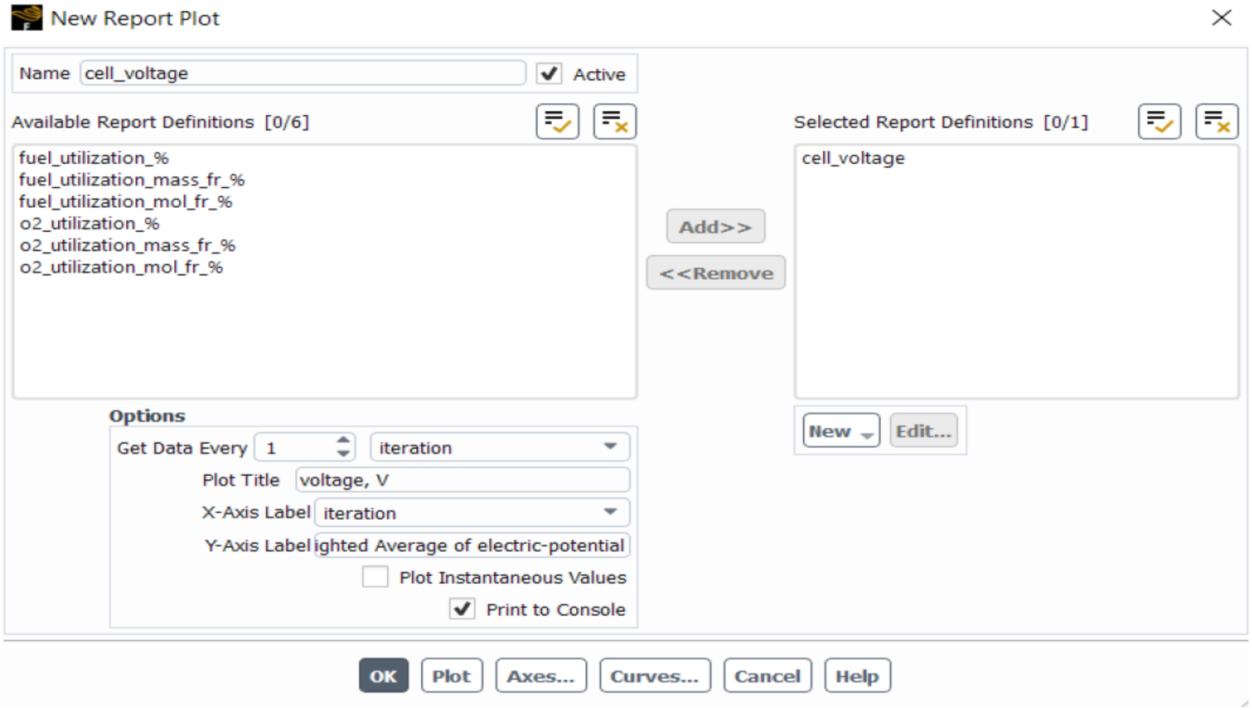
Selected Report Definitions [0/2]

fuel_utilization_mol_fr_%
o2_utilization_mol_fr_%

Options

Get Data Every 1 iteration
Plot Title h2_o2_utilization
X-Axis Label iteration
Y-Axis Label fuel_utilization,o2_utilization
☐ Plot Instantaneous Values
☑ Print to Console

Figure 11: Report plots for hydrogen and oxygen utilization



New Report Plot

Name cell_voltage ☑ Active

Available Report Definitions [0/6]

fuel_utilization_%
fuel_utilization_mass_fr_%
fuel_utilization_mol_fr_%
o2_utilization_%
o2_utilization_mass_fr_%
o2_utilization_mol_fr_%

Selected Report Definitions [0/1]

cell_voltage

Options

Get Data Every 1 iteration
Plot Title voltage, V
X-Axis Label iteration
Y-Axis Label ighted Average of electric-potential
☐ Plot Instantaneous Values
☑ Print to Console

Figure 12: Report definition for cell voltage

4.5 Results

Obtaining the polarization curve is not that simple and straight in case of Ansys Fluent, we have to run it for multiple current values in order to get the voltage, and then plotting it in Excel. For example – obtaining this curve below took almost 15 hours

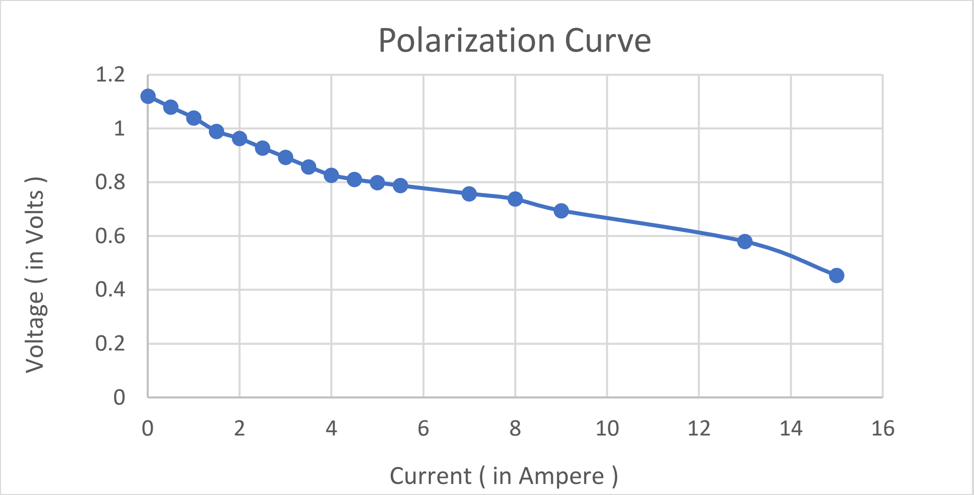


Figure 13: Voltage-current curve obtained by fluent

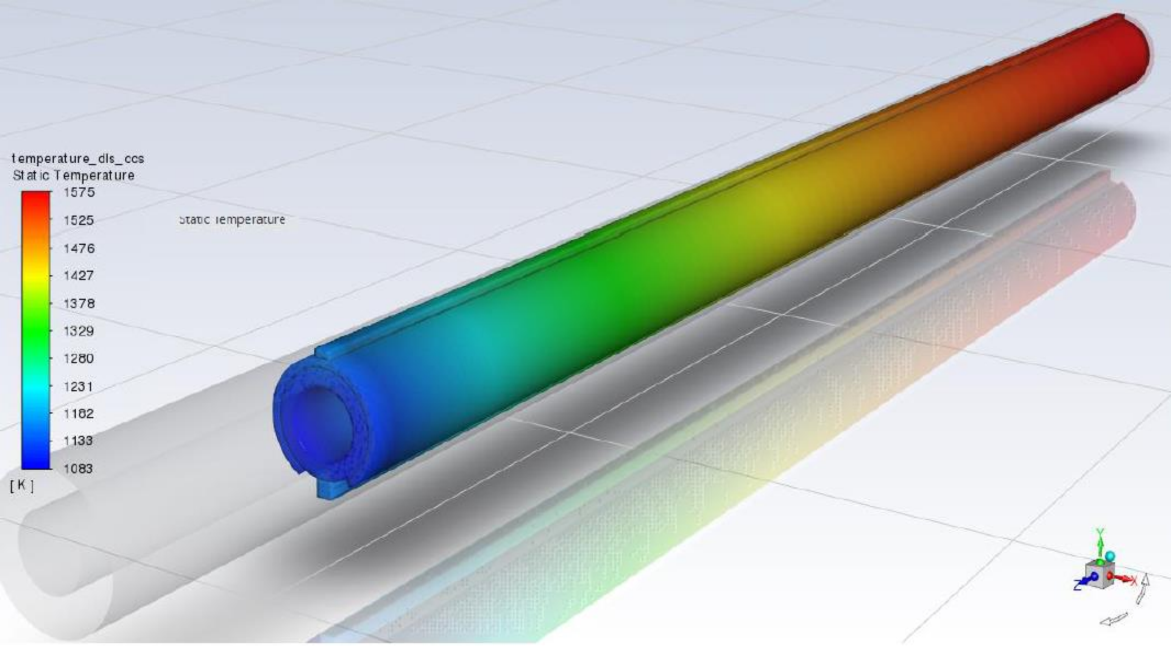


Figure 14: Temperature distribution on Anode and cathode

- The results indicate that the open circuit voltage was 1.1 Volts which then suffers losses such as activation polarization loss, then it suffered internal resistance to the flow of the current which resulted in ohmic losses and then it suffered very minor concentration losses due to mass transport.

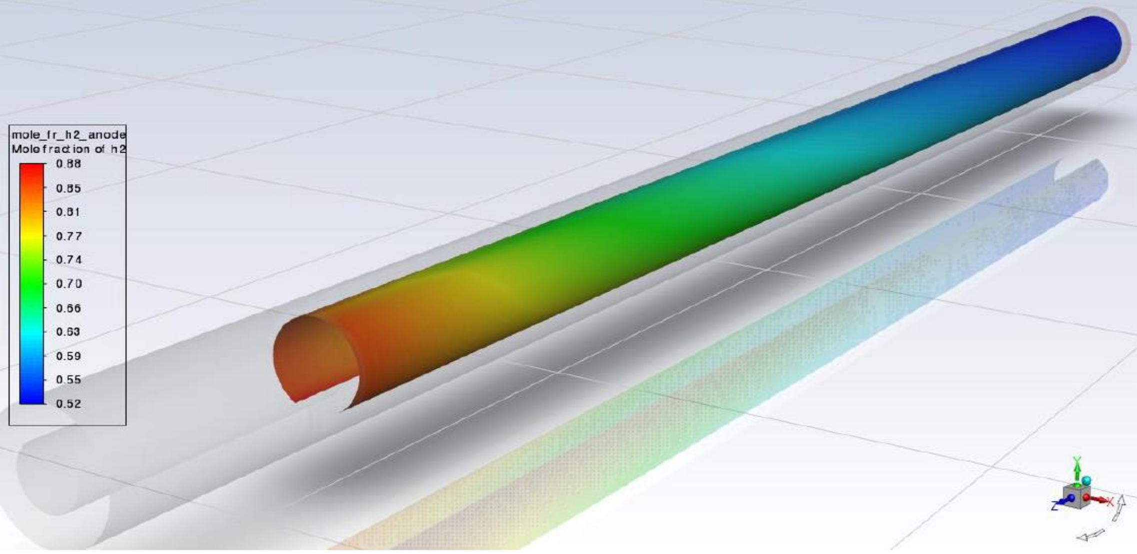


Figure 15: Mass fraction of hydrogen at anode side of electrolyte

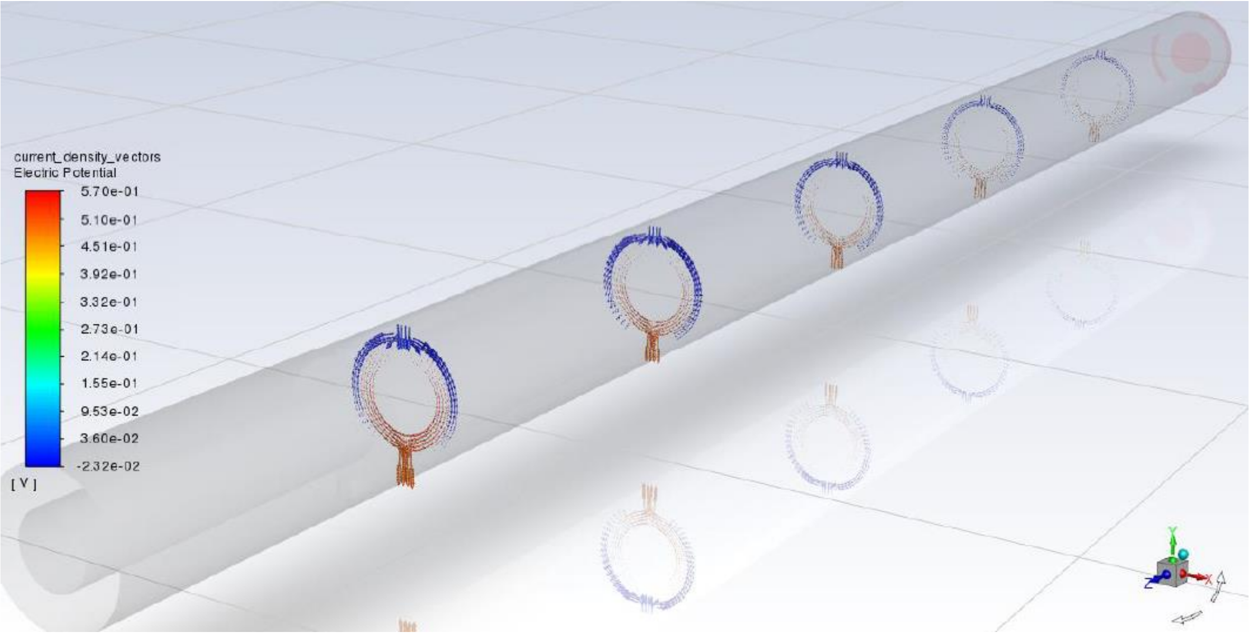


Figure 16: Current density vector distribution at cross sections

CHAPTER 5

Impact of Input parameters on the performance of Planar SOFC using COMSOL Multiphysics

5.1 COMSOL Multi-physics Capabilities

The software package is a versatile (FEA) solver and simulation software specifically designed to cater to a broad spectrum of physics and engineering applications. It excels in handling coupled phenomena or multiphysics simulations, where multiple physical phenomena interact with each other. The software enables users to analyze and simulate complex systems, considering the interactions between different physics domains, such as structural mechanics, fluid dynamics, heat transfer, electromagnetics, and more. Its capabilities make it suitable for solving diverse engineering problems and optimizing designs in various industries and research fields.

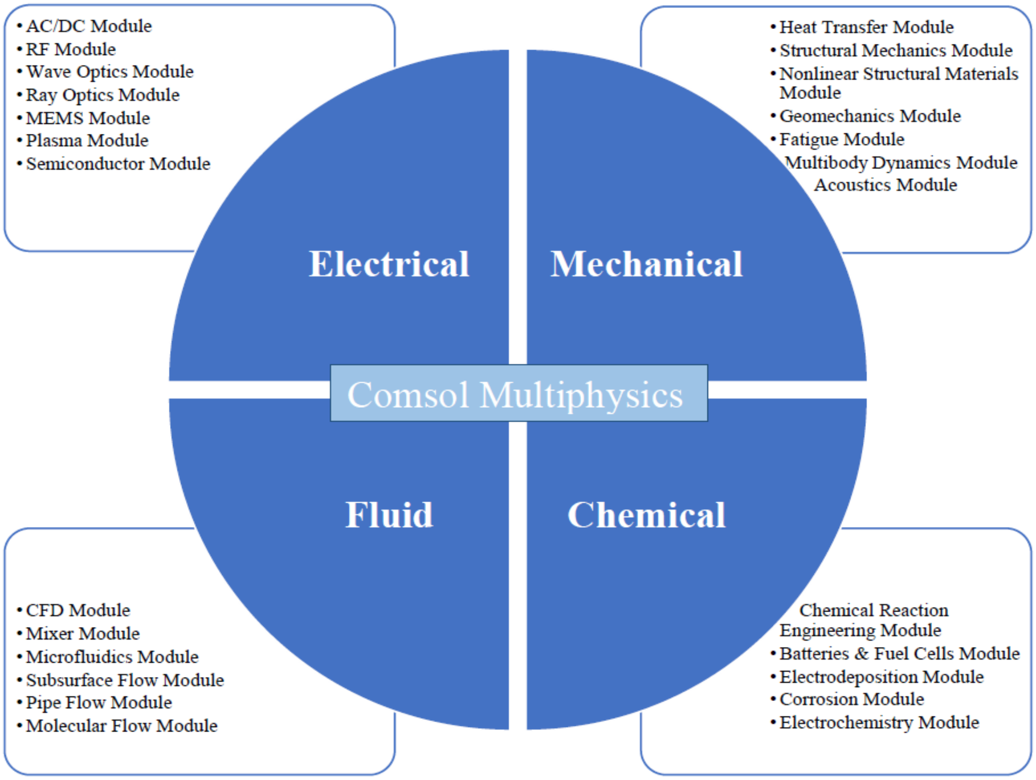


Figure 17: Modules in COMSOL [courtesy-COMSOL]

5.2 COMSOL Multiphysics process flow

COMSOL Multiphysics follows a structured approach consisting of eight steps to create a study

Step 1. Model.
Step 2. Definitions.
Step 3. Geometry.
Step 4. Materials.
Step 5. Physics.
Step 6. Mesh.
Step 7. Study.
Step 8. Results

5.3 Losses associated with Fuel Cells

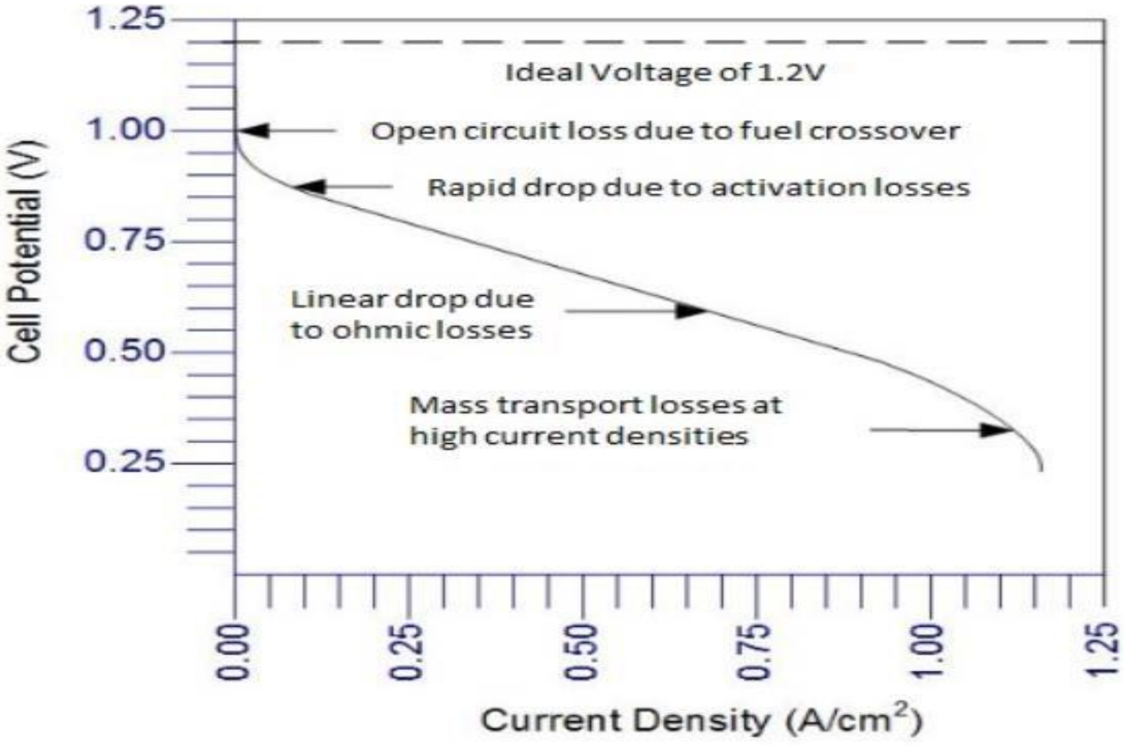


Figure 18: Loss of Energy in Fuel Cells

5.3.1 Activation Polarization losses

- Activation polarization is the voltage over potential required to overcome the activation energy of the electrochemical reaction on the catalytic surface
- Dominates losses at low current density

- In high-temperature fuel cells, the operating temperatures are so high that the activation losses are very low.

$$\Delta \mathrm{V_{act}} = \mathrm{E_r} - \mathrm{E} = \frac{\mathrm{RT}}{\mathrm{\alpha F}} \ln \frac{\mathrm{i}}{\mathrm{i_0}}$$

- ΔV_{act} = Loss in Potential with activation
- F= faraday's constant
- E_r = Reversible open circuit voltage (Theoretical value)
- E= Actual Open circuit voltage
- α = charge transfer coefficient
- R = Universal gas constant
- i = actual Current
- i_0= Open circuit current
- T= Temperature

5.3.2 Ohmic Polarization losses

It comes from intrinsic resistance to charge flow in Conductors

• Ohmic losses includes electronic (R elec) and ionic (R ionic) contributions to fuel cell resistance

$$v_{ohmic} = iR_{ohmic} = i(R_{elec} + R_{ionic})$$[8]

$\mathrm{v_{ohmic}}$= Ohmic polarization losses

$\mathrm{R_{ohmic}}$ = Ohmic resistance

$\mathrm{R_{ionic}}$= Ionic resistance

$\mathrm{R_{elec}}$=Electronic resistance

5.3.3 Concentration Polarization losses

Concentration polarization occurs when the concentration of a specific component increases or decreases at the boundary layer close to the membrane surface due to the selective transport through the membrane

$$v_{ohmic} = c \ ln \frac{i_L}{i_L - i}$$ [8]

where c is a constant

$c = \frac{RT}{nF}\left(1 + \frac{1}{\alpha}\right)$ where n = number of free electrons participating in the reaction

5.3.4 Actual Energy left after losses

$$V(i) = V_{rev} - v_{act_{anode}} - v_{act_{cath}} - v_{ohmic} - v_{conc\_anode} - v_{conc\_cath}$$

Where

V_{rev}	Reversible voltage (Theoretical)
$v_{act_{cathode}}$	Activation loss at cathode
$v_{act_{anode}}$	Activation loss at anode
v_{ohmic}	Ohmic losses due to resistance
v_{conc_anode}	Concentration losses at anode
v_{conc_cath}	Concentration losses at cathode

5.4 Model Description

In this study, we considered a Planar SOFC with counter flow configuration. Thereafter this study will certainly help in the understanding the basics of Cell level modeling and thus help in optimization of cell performance by studying the impact of various input parameters like pressure, temperature, Gas diffusion electrode porosity, Cell length and Electrode thickness

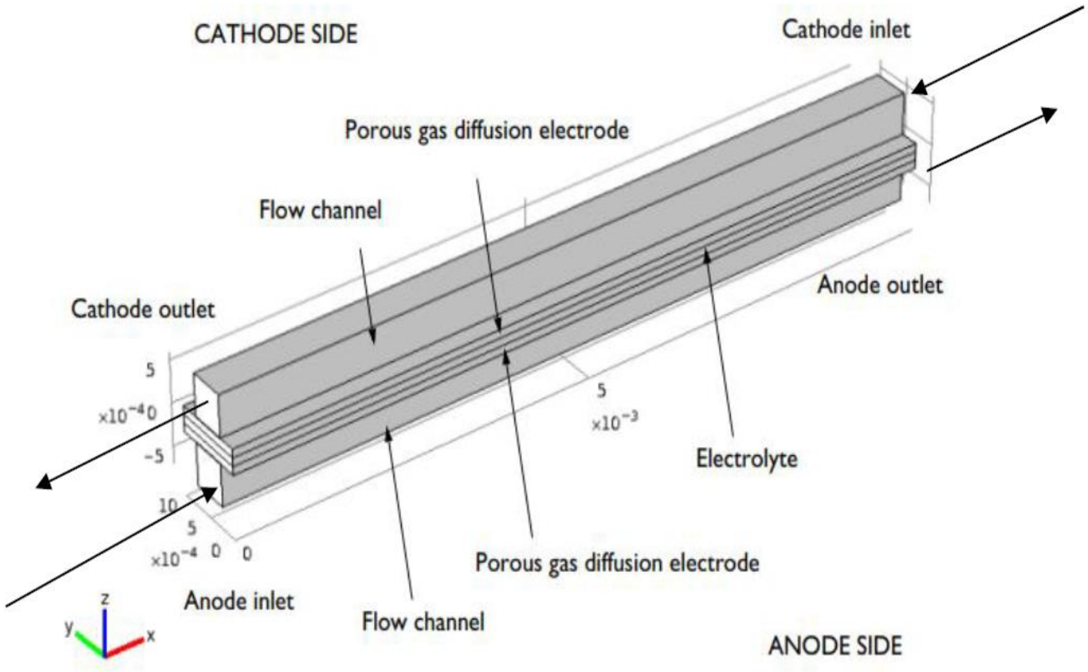


Figure 19:[Screenshot] Planar SOFC[12]

Table 1: Geometrical Parameters

Geometrical Parameters	**Value (in meter)**
Gas flow channel width	5.00E-04[m]
Rib width	5.00E-04[m]
Gas diffusion electrode thickness	1.00E-04[m]
Electrolyte thickness	1.00E-04[m]
Gas flow channel height	5.00E-04[m]
Flow channel length	1.00E-02[m]
Height of Cathode Gas diffusion layer	1e-4[m]
Height of Anode Gas Diffusion Layer	1e-4[m]

Table 2: Chemistry Parameters

Chemical Parameters (independent)	**Value**
Molar mass, H_2	2[g/mol]
Molar mass, O_2	32[g/mol]
Molar mass, N_2	28[g/mol]
Molar mass, H_2O	18[g/mol]
Reference diffusivity	$3.16e-08[m^2/s]$
Inlet weight fraction, H_2 at anode	0.4
Inlet weight fraction, O_2 at cathode	0.15
Inlet weight fraction, H_2O at cathode	0.37

Table 3: Electrical Parameters

Electrical Properties	**Value**
Exchange current density, anode	0.1[A/m^2]
Exchange current density,cathode	0.01[A/m^2]
Initial cell polarization	0.05[V]
Equilibrium voltage, anode	0[V]
Equilibrium voltage, cathode	1[V]
Cell voltage	$\mathrm{E_{eq\_c} - E_{eq\_a} - V_{pol}}$
Electrolyte effective conductivity,anode	1[S/m]
Solid effective conductivity,anode	1000[S/m]
Electrolyte effective conductivity,cathode	1[S/m]
Solid effective conductivity,cathode	1000[S/m]
Electrolyte conductivity	5[S/m]
Current collector conductivity	5000[S/m]

Table 4: Physical parameters

Physical Parameters	**Value**
Atmospheric pressure	1[atm]
Temperature	600[degC]
Viscosity, air	3.00E-05[$Pa \times s$]
Pressure drop, anode	2[Pa]
Pressure drop, cathode	6[Pa]
Anode permeability	1.00E-10[m^2]
Cathode permeability	1.00E-10[m^2]
Porosity	0.4
SSA, anode	1.00E+09[1/m]
SSA, cathode	1.00E+09[1/m]
Kinetic volume, H_2	0.000006
Kinetic volume, O2	0.0000166
Kinetic volume, N2	0.0000179
Kinetic volume, H_2O	0.0000127

5.5 Assumptions used:

- Surface-to-surface radiation between internal boundaries is neglected
- Model considers electronic conduction between electrodes
- Electrochemical reactions happening at the triple phase boundary only
- Ionic conduction only in the electrolyte
- Mass transport dominates in porous electrodes

5.6 Methodology

Select New Wizard
(Open COMSOL and go to New Wizard > 3D)

⇩

Select Physics
- Secondary current distribution
- Transport of concentrated species for both cathode and anode
- Free and porous media flow for both cathode and anode

⇩

Specify parameters

- mass fractions in transport of concentrated species
- Velocity parameters (must be unique for cathode and anode)

Specify study type
(Stationary (steady case) for this study)

Specify all parameters in .txt file and load as parameters

- Geometrical Parameters
- Electrical Parameters
- Chemical Parameters
- Physical Parameters

Specify the geometry

- Take Work plane and add rectangles
- Specify the geometrical entities as a parameter

Define Explicit Definitions (for easy and fast selection)

- Defining Cathode Gas Diffusion layer
- Defining Anode GDL
- Defining Flow channels for both anode and cathode

Defining Boundary probe

- A boundary probe is given at electrolyte- anode diffusion layer interface for measuring average current density for the final polarization curve

Setup Secondary current distribution module

- Anode GDL
- Cathode GDL
- Electrolyte

Specify porous electrode

Define

- Cathode gas diffusion electrode
- Anode gas diffusion electrode
- define porosity
- chemistry & mass transfer

Setup Transport of concentrated species at cathode and anode

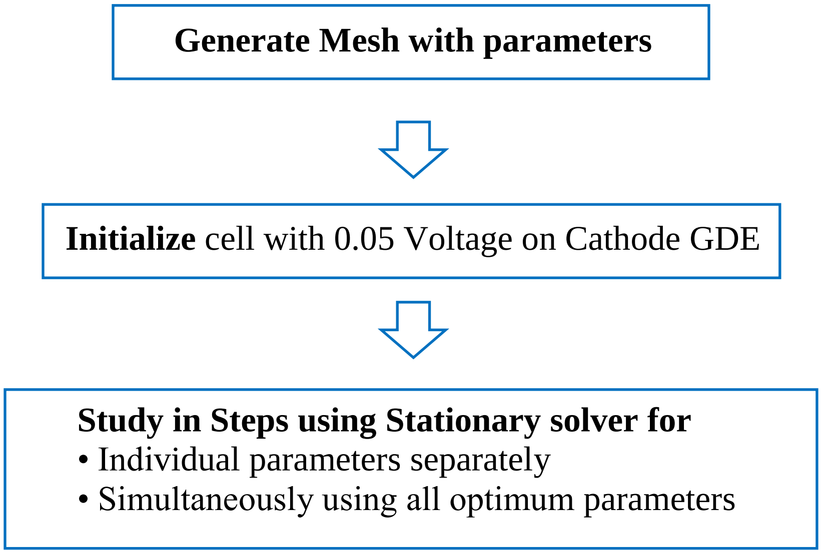
- Define Diffusion and convection values (Maxwell-Stefan diffusion model used in this case)
- Defining reaction coefficients for coupling of porous electrode
- Define Inflow and outflow mass fractions and location at cathode and anode channels

Setup Free and porous media flow

- Specify CFD flow properties for both anode and cathode flow channels
- Define Stoichiometric conditions
- Specify Compressibility conditions (here Mach<0.3)

Couple Multiphysics

- Electrical part, chemical part and CFD part



5.7 Modeling Approach

- In the present simulation methodology, gas diffusion electrode layers, flow channels and electrolyte are modelled as a planar cross flow configuration. The Cathode and anode current collectors are not modelled as such, but their condition have been specified at the top and bottom of the flow channels.
- At the Cathode side we considered species such as Nitrogen and oxygen will flow along with a mixture of small amount of water.
- At the Anode side pure Hydrogen and water vapor mixture will flow in the opposite direction to the air flow

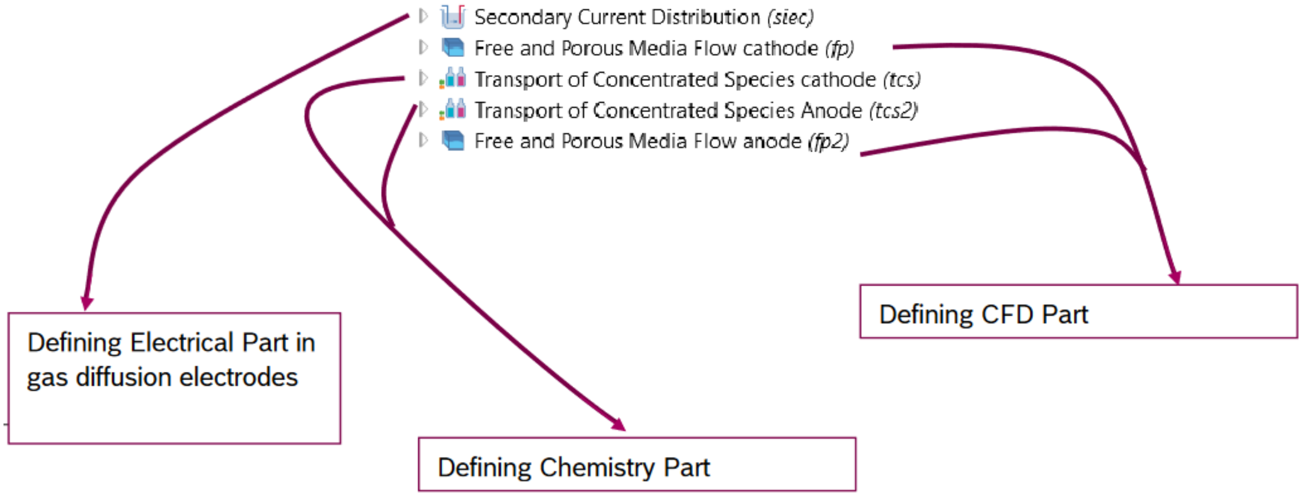


Figure 20: Modules used for study

5.8 Boundary Conditions

There are multiple type of physics boundary conditions like electrical boundary condition and cfd boundary conditions, apart from this chemical boundary conditions are also required

5.8.1 Electrical Boundary conditions

- The flow of oxygen ions should start from cathode to anode. For that an equilibrium voltage potential of 1 Volts was applied at the cathode and a ground condition was given at the anode.
- An exchange current density of 0.1 A/m^2 was assigned to the anode, while a value of 0.01 $A/m^2$was assigned to the cathode.
- ECD represents the rate of oxidation and reduction at equilibrium electrode.

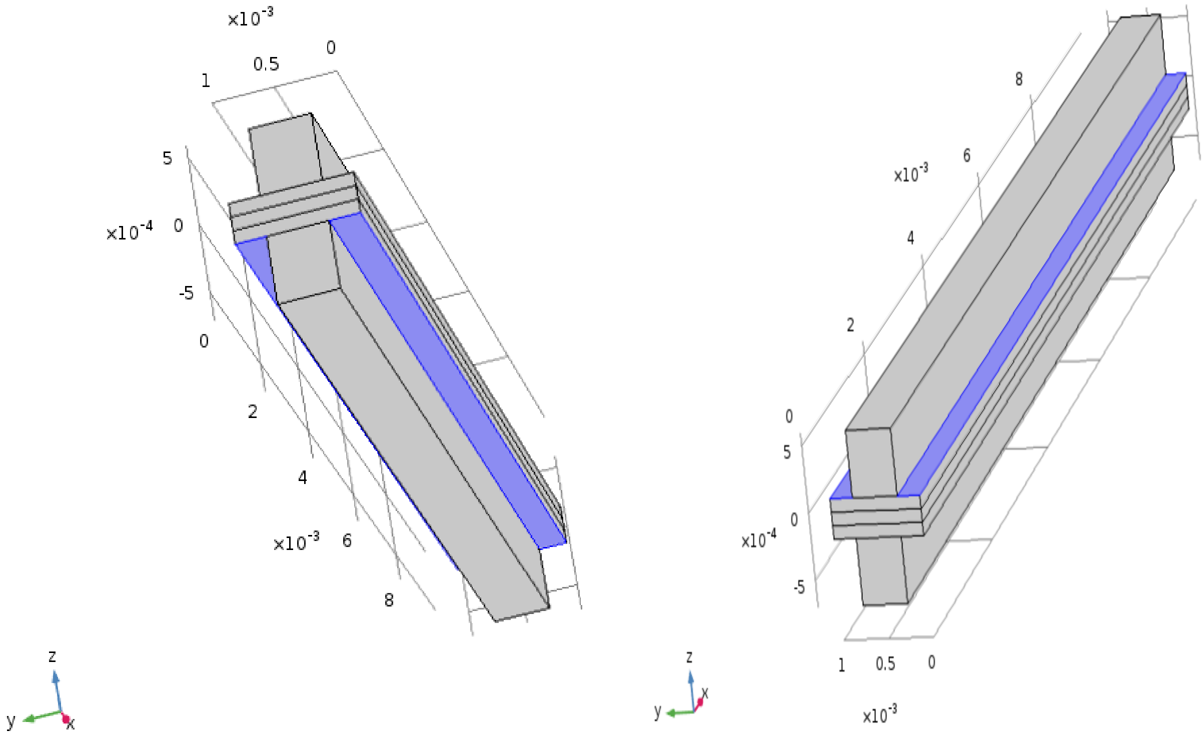


Figure 21: Electric ground and electrical potential boundary conditions

5.8.2 Defining CFD & Chemical Boundary Conditions

- At the cathode flow channel, as air is there we have given a pressure drop boundary condition of 6 pascal and at the anode side we have provided a condition of 2 Pascals.

- In the gas diffusion electrodes, a porosity of 40 % was taken for both cathode and anode GDE.
- The temperature of 600 degree Celsius was provided as the minimum temperature input for the model. In the beginning the atmospheric pressure taken was 1 atm which was gradually increased for parametric study.
- Inlet weight fraction of 0.4 was taken at the anode. Inlet weight fraction for oxygen at the cathode was taken as 0.15 and inlet weight fraction for water was 0.37.The molar mass for all species are taken from the chemistry.
- The specific surface area at anode and cathode also was taken as 1e+9 [1/m]
- The reference diffusivity was taken as 3.16e-08 m^2/sec. The viscosity of air was taken as 3e-5 Pa*sec

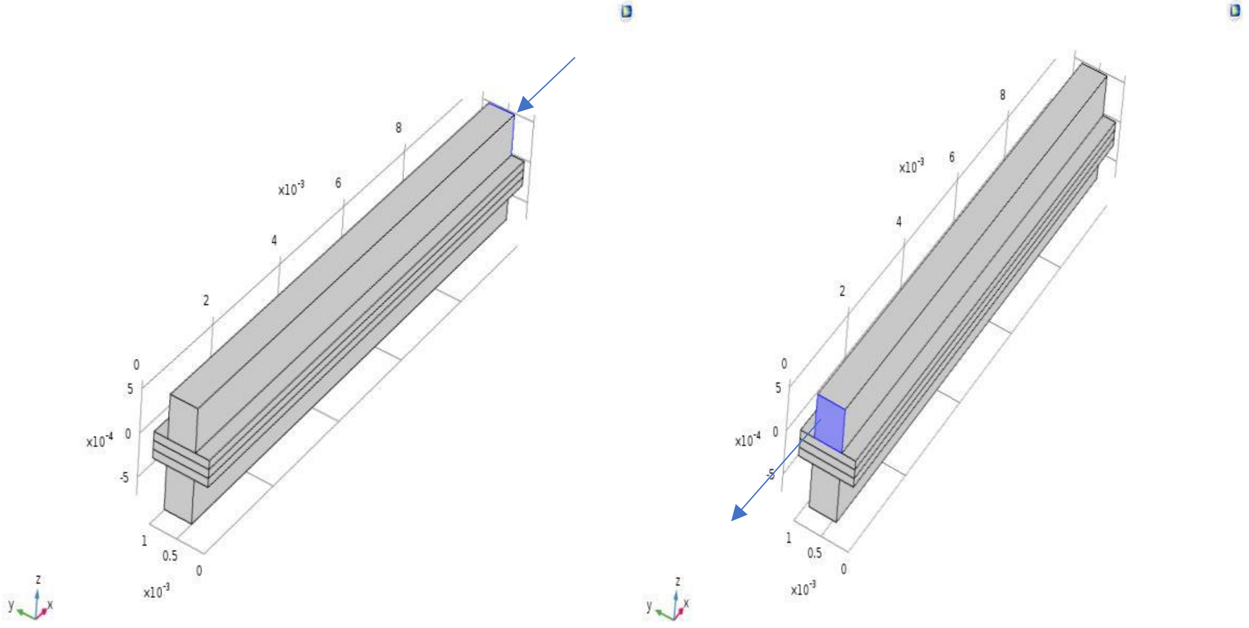


Figure 22: Inlet and outlet position for air at cathode flow channel

- Maxwell Stefan diffusion matrix is used to define diffusivities
- Diffusivity is to be defined in gas flow channels where hydrogen and air will flow in cross flow configuration
- Effective diffusivity is to be defined in the gas diffusion electrode layers only because the mixture rate should be higher in them.

5.8.3 Meshing Approach

- Mesh has a huge impact on the solving time in COMSOL because the problem which looks so simple but when it got coupled with Multiphysics, it become highly intensive for an FEM solver

- For this approach, mostly hexahedral elements are taken, and coarse regions were given to the areas like flow channels and fine regions were given on gas diffusion electrodes.

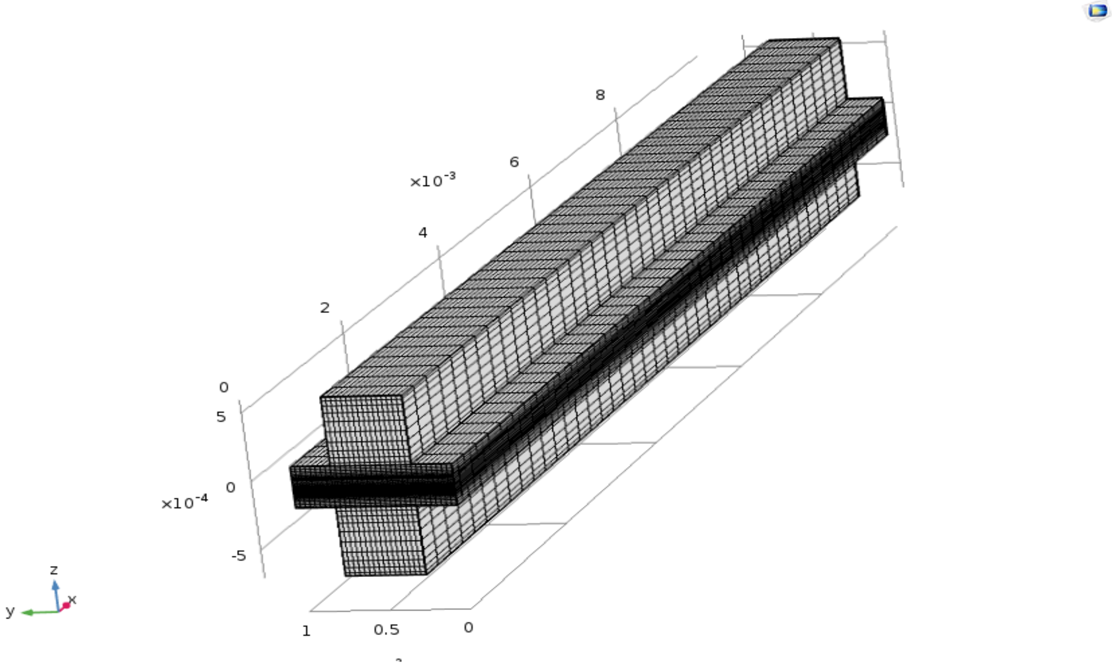


Figure 22.1: Meshing of SOFC

- The finest regions were specified to the electrolyte where the physics and chemistry capture is critical.
- A parametric mesh is specified so that we don't have to mesh again on the geometry change.
- A mapped mesh approach has been considered for this case where the maximum element size taken as a parameter ($Width\ of\ channel\ /\ 8$) and the mesh is calibrated for Fluid dynamics in general mesh settings.
- Complete mesh consists of 57600 domain elements, 13680 boundary elements, and 1180 edge elements

5.9 Results and Discussion

5.9.1 Impact of Atmospheric pressure on Performance of SOFC Cell

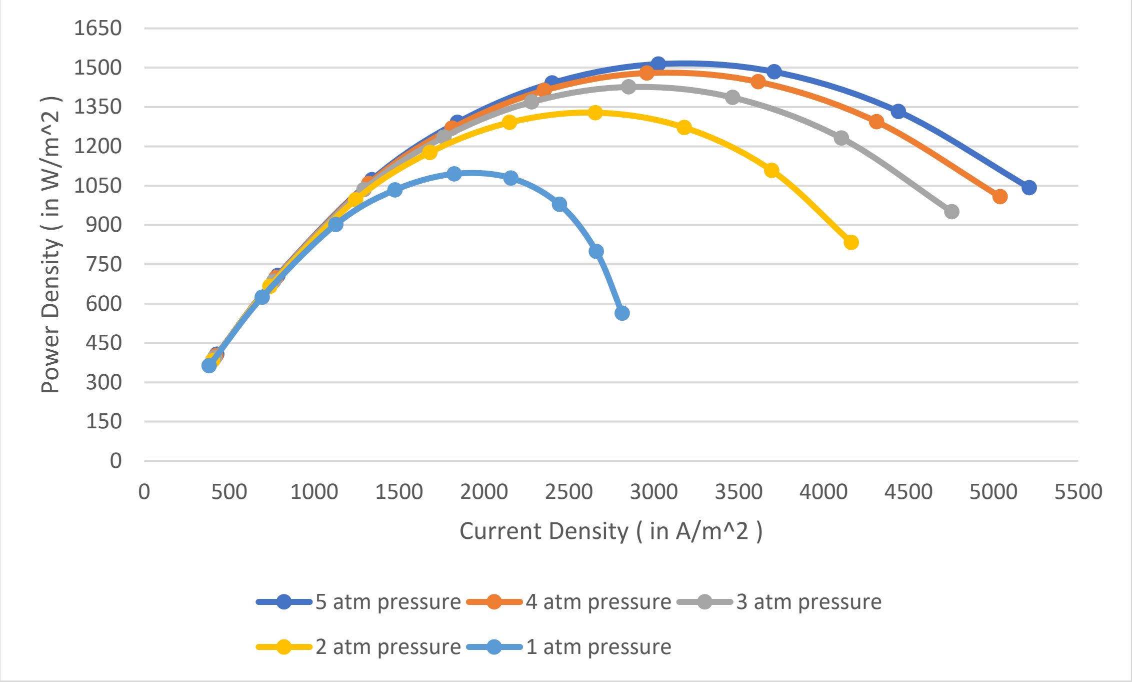


Figure 23: Impact of atmospheric pressure on sofc power density

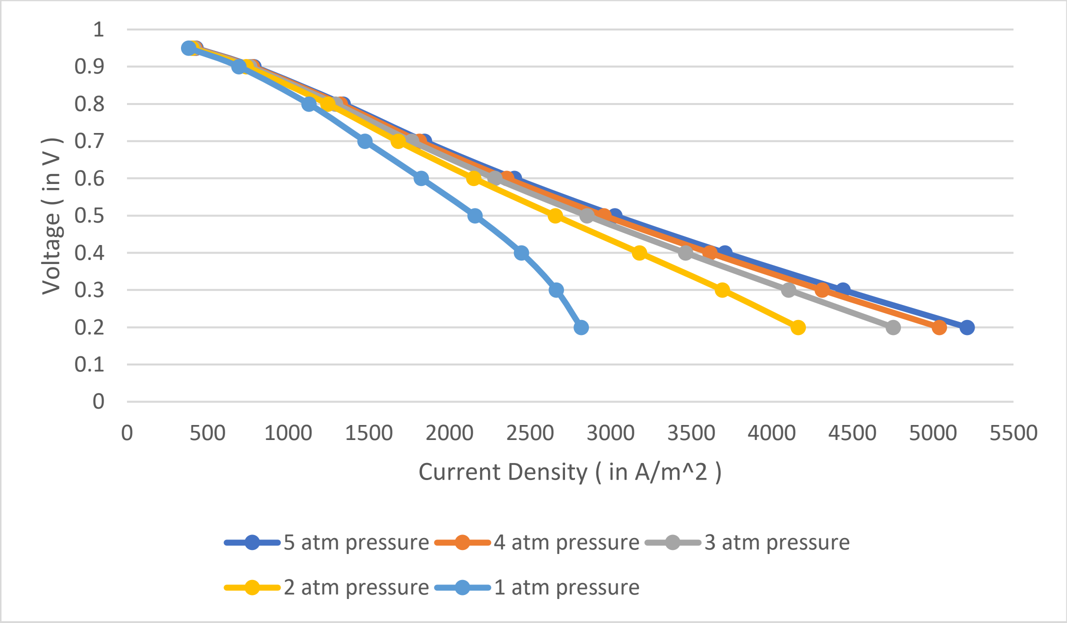


Figure 24: Impact of atmospheric pressure on polarization curve

- As we increased the atmospheric pressure ranging from 1 atm to 5 atm , we noticed that the maximum power density curve trends to be increasing along with the average current density
- This trend for pressure is same as obtained by various testing data obtained from carious research papers like [14] and [15]
- The same trend is seen for the Polarization curve also where OCV remains the same but the average current density is in the increasing trend

Therefore, we can conclude that the simulation results trend is matching with the testing data obtained from various research papers like the figure below

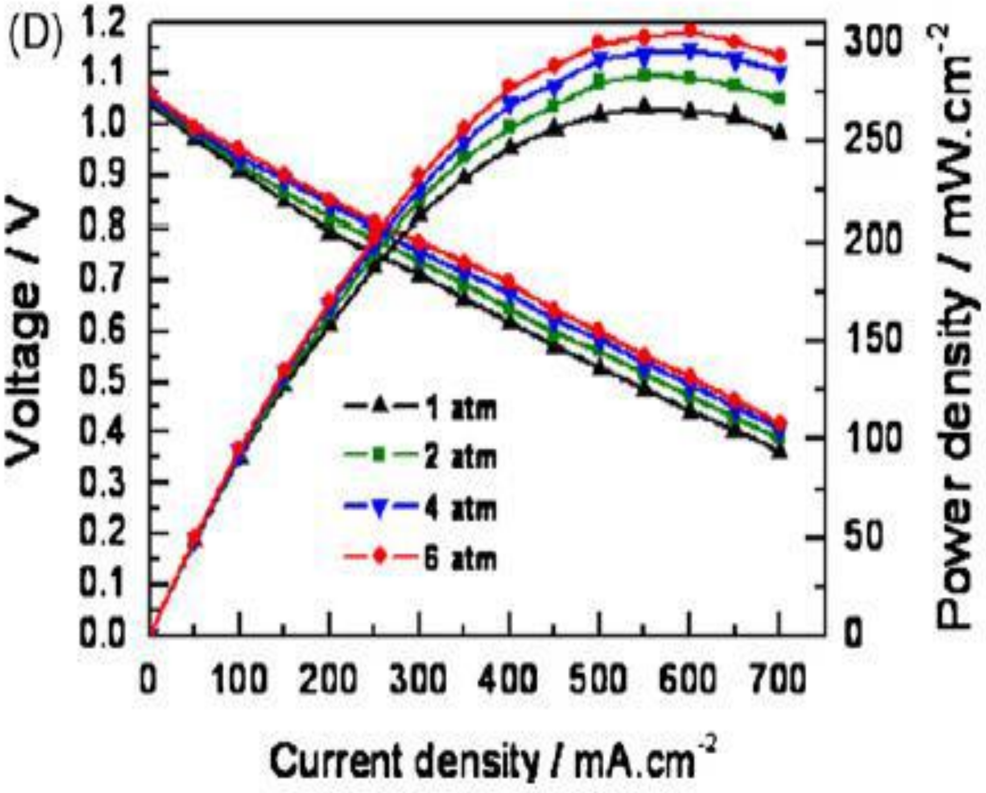


Figure 25- Trend from sofc testing data with different operational parameters [14]

5.9.2 Impact of Temperature on Performance of SOFC Cell

- The temperature is varied from 600 degree Celsius to 1000 Celsius with the increment of 100 for this study.
- The impact of temperature possesses a different trend as compared to testing data. This could be because of the impact of other operational parameters dominating the effect thereby reducing the overall effect of individualized effect of temperature.

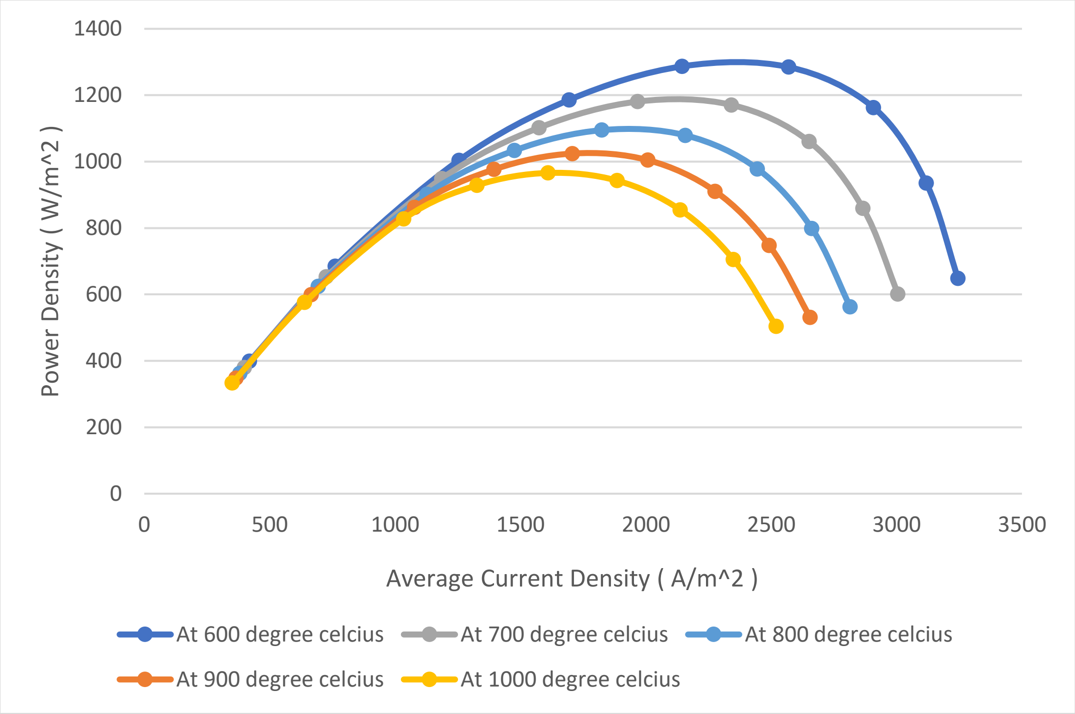


Figure 26: Impact of temperature on SOFC power density

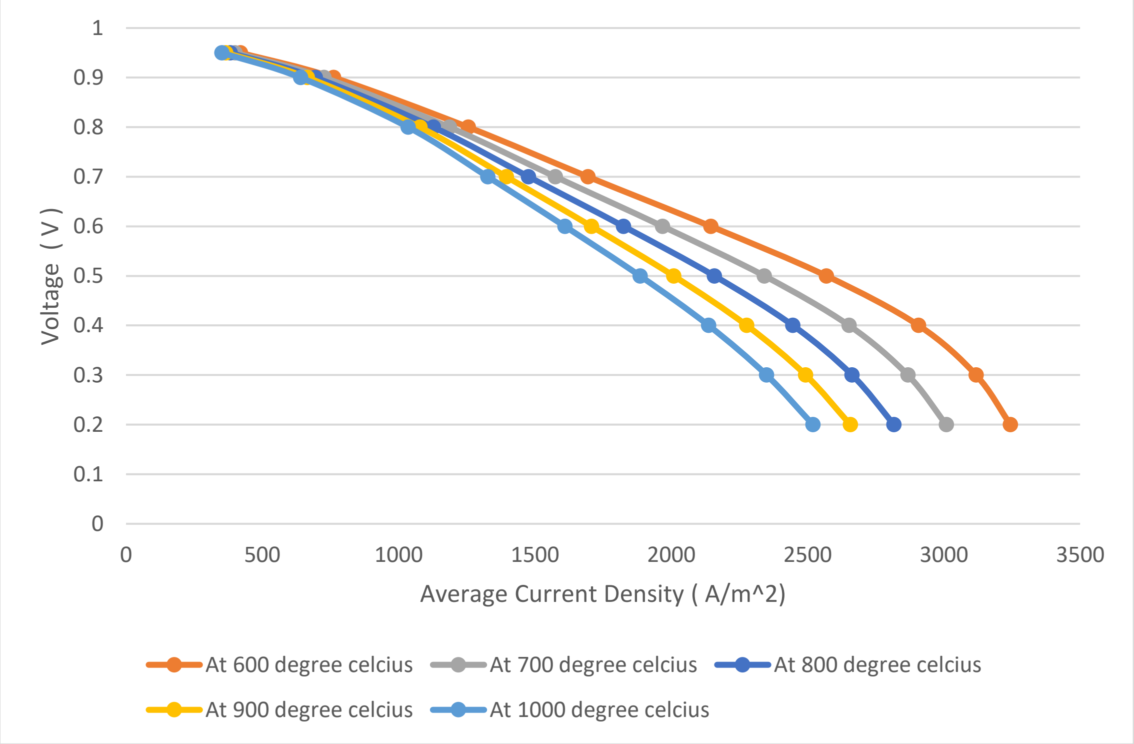


Figure 27: Impact of temperature on polarization curve

5.9.3 Impact of Gas diffusion layer porosity on Performance of SOFC Cell

- In this study, gas diffusion porosity is varied from 20% to 40% for the gas diffusion electrodes like Cathode GDE and anode GDE
- The impact on performance was minimal as compared to other operational parameters. At 40% porosity peak power density was observed to be the highest and at 20 % it was the lowest. Same trend is observed for average current density
- Electrolyte is modelled as a solid wall with the properties specified like ionic and electrical conductivities and is assumed to be isotropic material configuration for the simplicity of this study
- The thickness which was specified as a parameter was varied from 15 microns to 100 microns with a multiple of 2x
- At the minimum thickness, that is 15 microns the power density and current density was coming out to be the highest

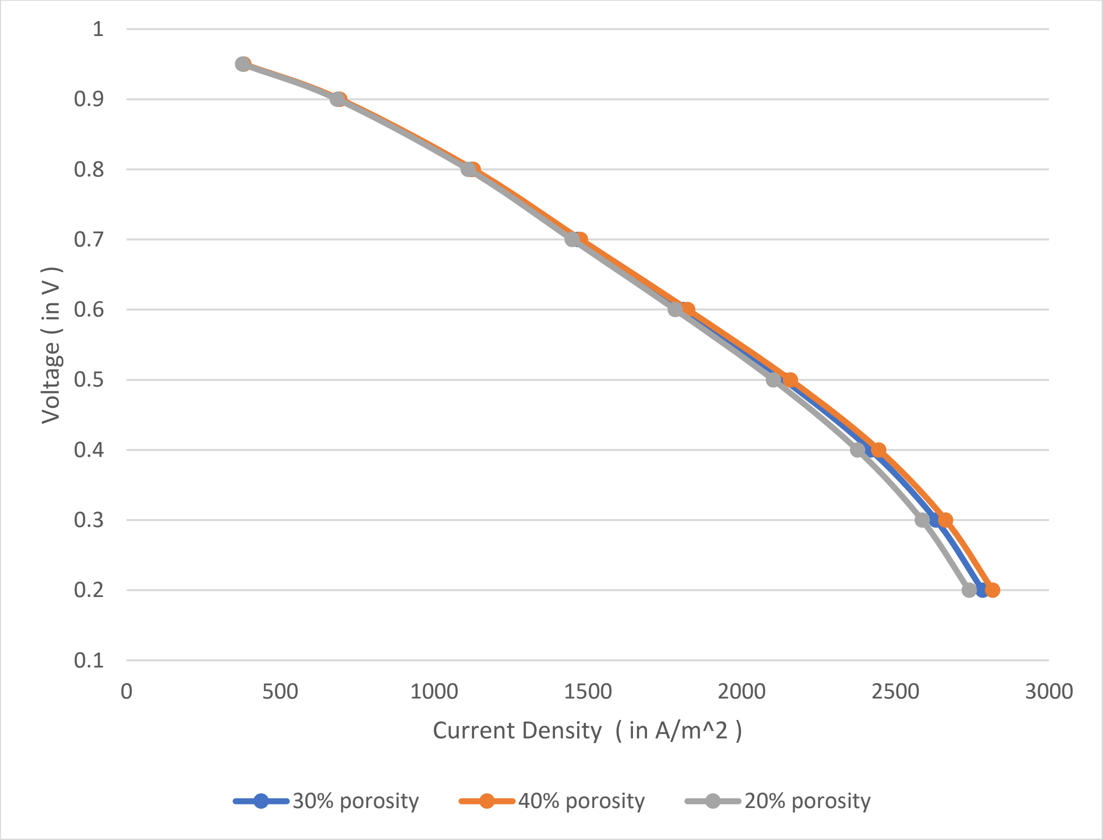


Figure 28: Impact of gas diffusion electrode porosity on polarization curve

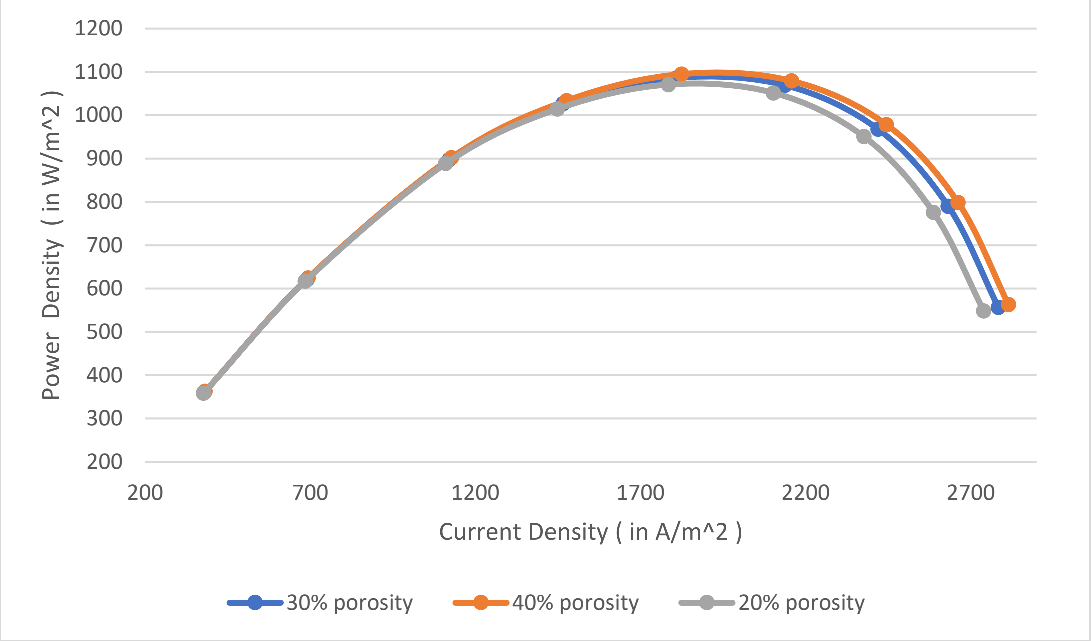


Figure 29: Impact of gas diffusion electrode porosity on power density

5.9.4 Impact of Electrolyte thickness on SOFC performance

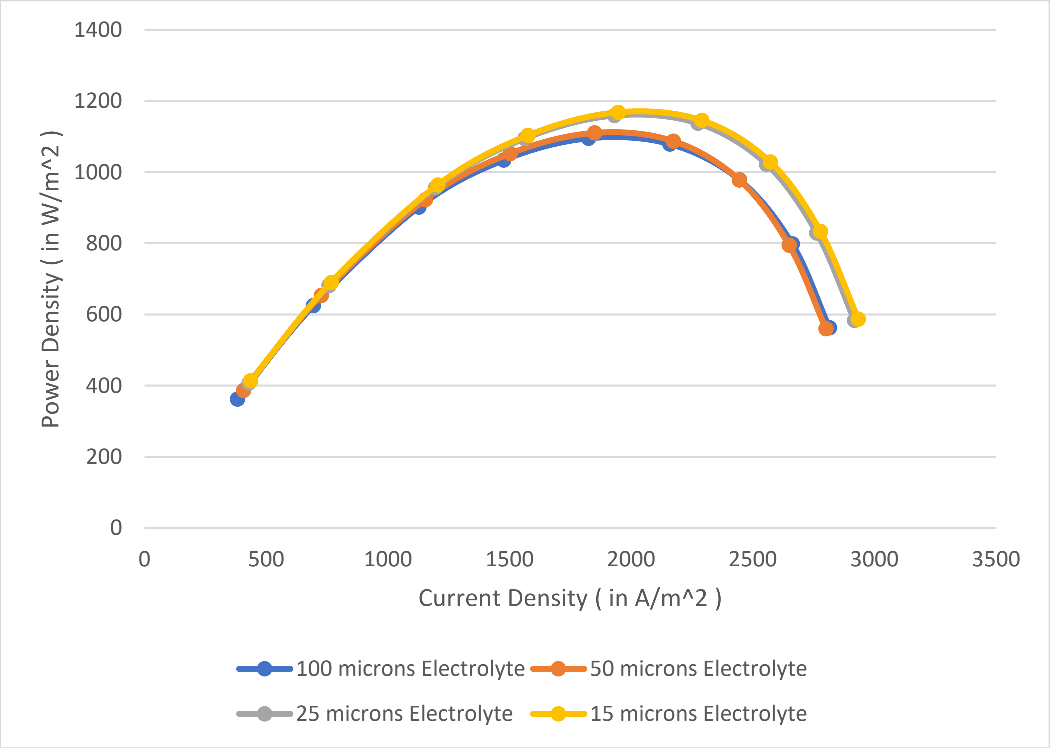


Figure 30: Impact of electrolyte thickness on SOFC performance

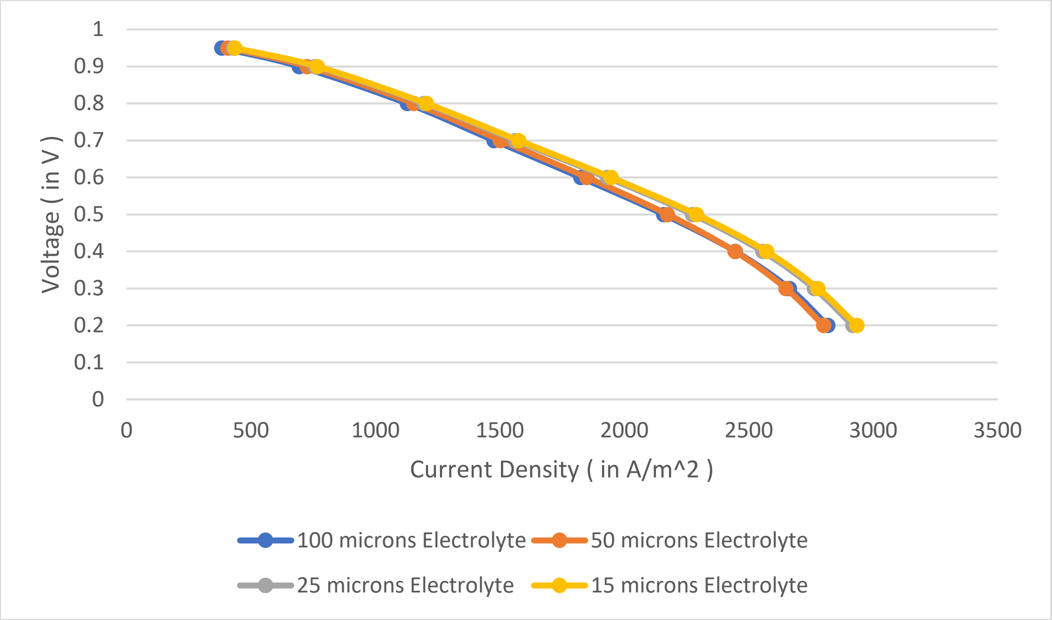


Figure 30: Impact of electrolyte thickness on SOFC performance

- Electrolyte is modelled as a solid wall with the properties specified like ionic and electrical conductivities and is assumed to be isotropic material configuration for the simplicity of this study
- The thickness which was specified as a parameter was varied from 15 microns to 100 microns with a multiple of 2x
- At the minimum thickness, that is 15 microns the power density and current density was coming out to be the highest

5.9.5 Impact of Cell length on SOFC Performance

- The original cell length of the cell in this case was 10 mm and for studying its impact its value is reduced to half i.e. 5 mm
- There is about 40% peak power increment just by reducing the cell length to half
- This could be because most of the hydrogen is getting consumed in the beginning of the cell and because we are measuring performance per unit area, so ultimately in full length, our per unit cell area is getting increased, so utilization is getting reduced in full length of the cell
- The thickness which was specified as a parameter was varied from 15 microns to 100 microns with a multiple of 2x
- Electrolyte is modelled as a solid wall with the properties specified like ionic and electrical conductivities and is assumed to be isotropic material configuration for the simplicity of this study

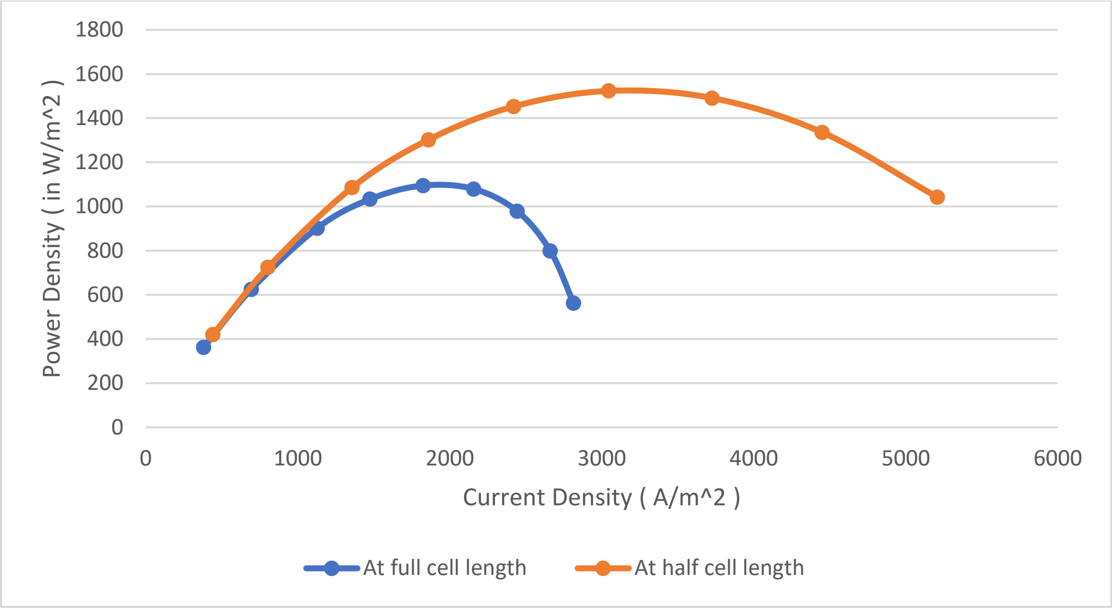


Figure 31: Impact of cell length in power density

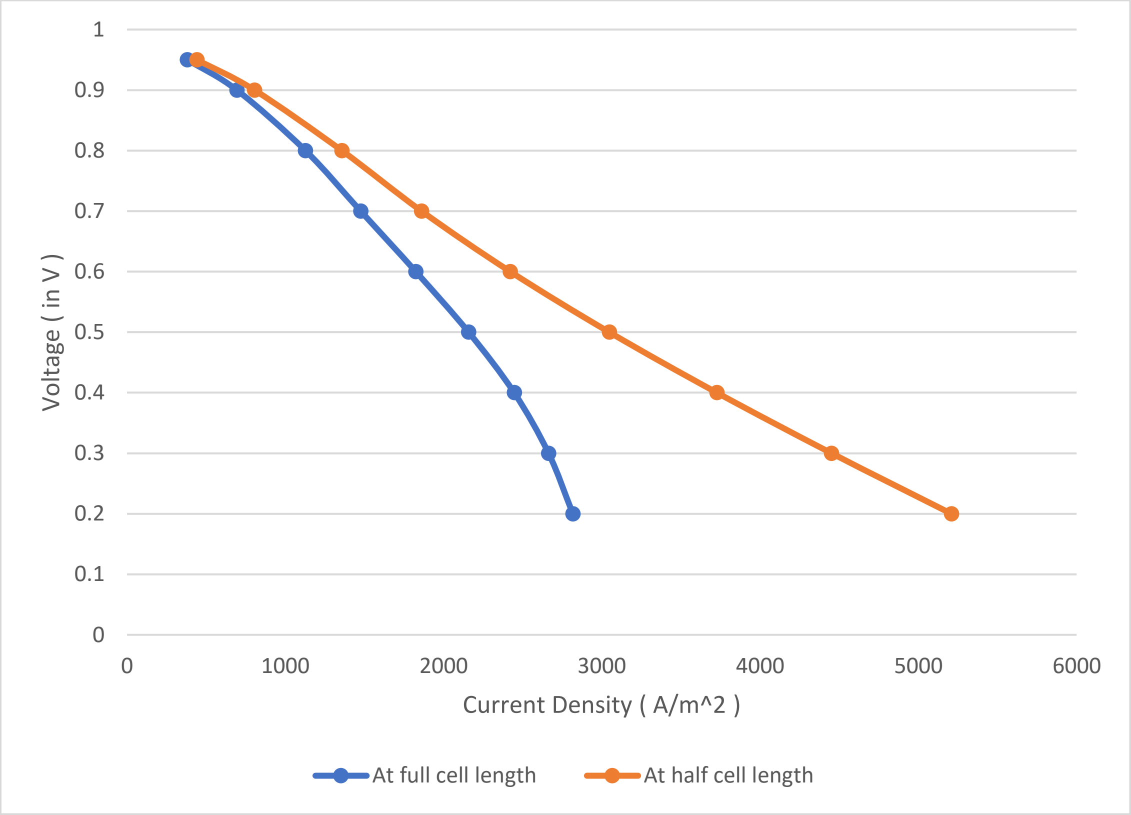


Figure 32: Impact of cell length on polarization curve

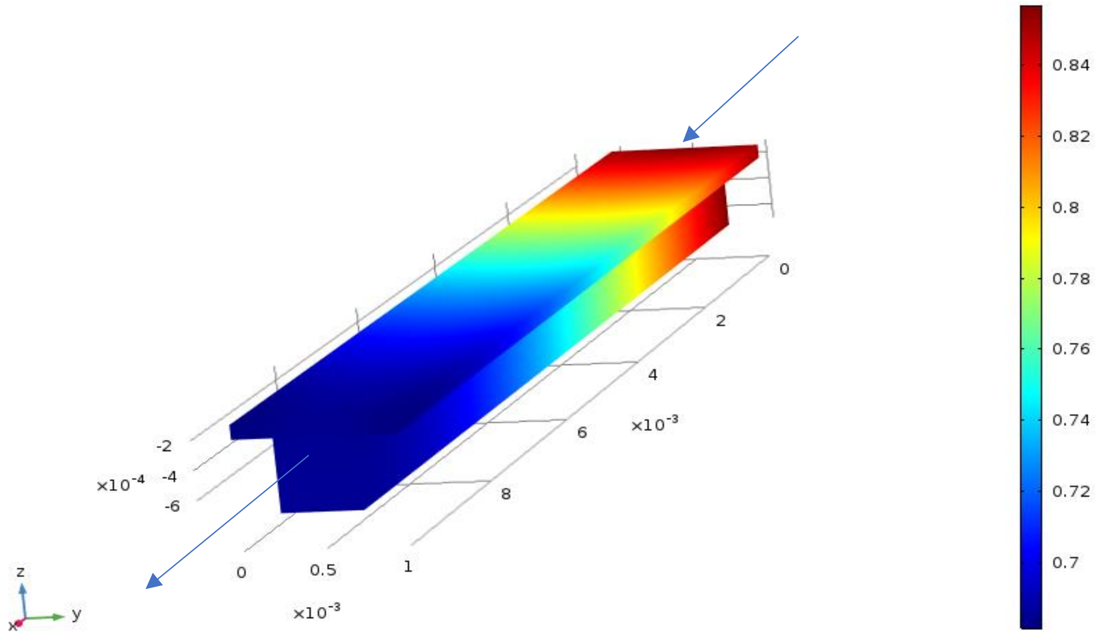


Figure 33: Mole fraction of hydrogen at anode

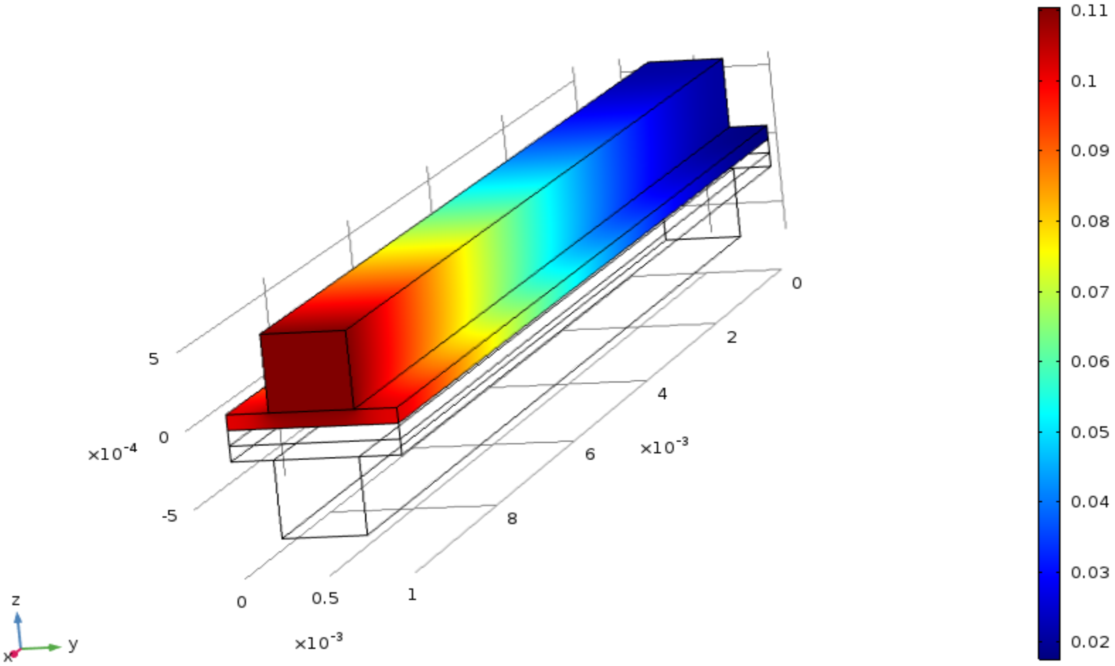


Figure 34: Mole fraction of oxygen at cathode

5.9.6 Mass Fraction of species:

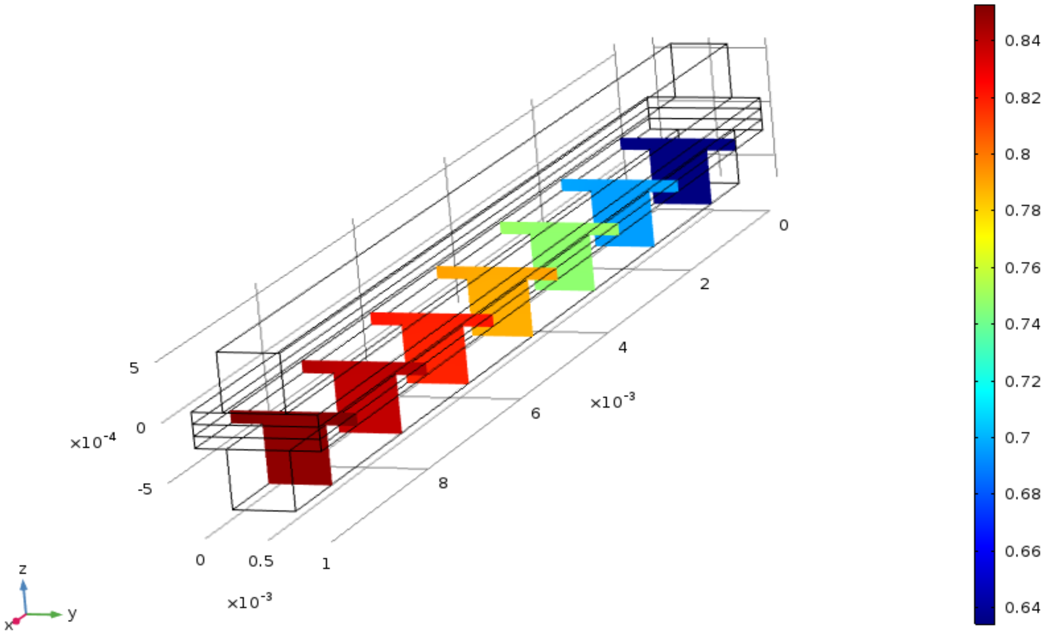


Figure 35: Mass fraction of water at anode

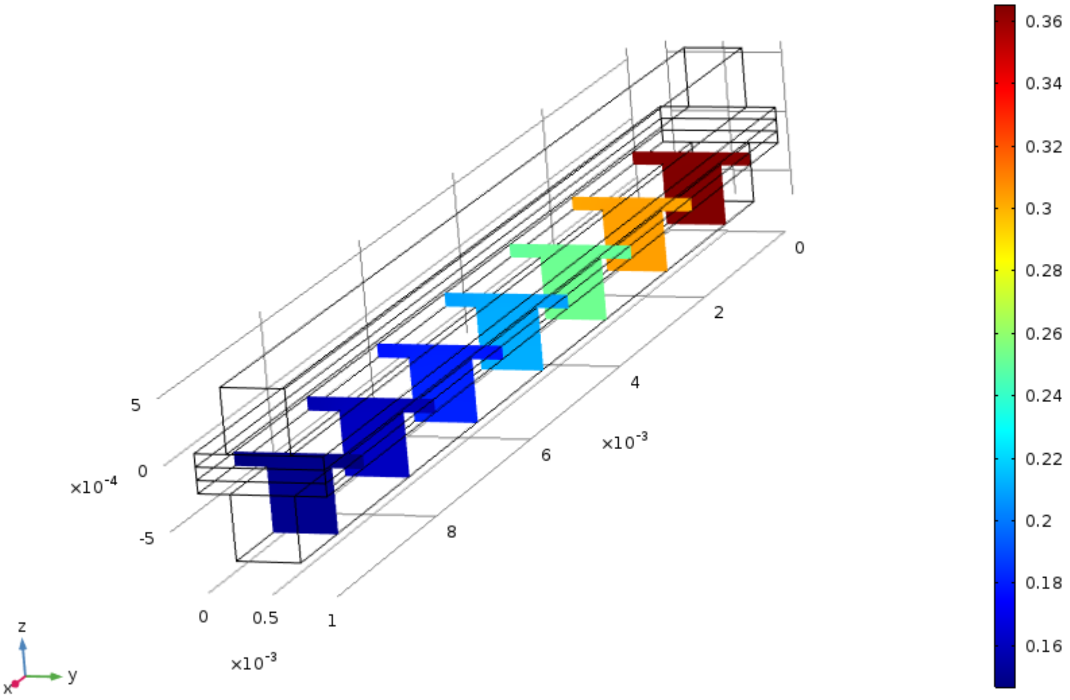


Figure 36: Mass fraction of hydrogen at anode

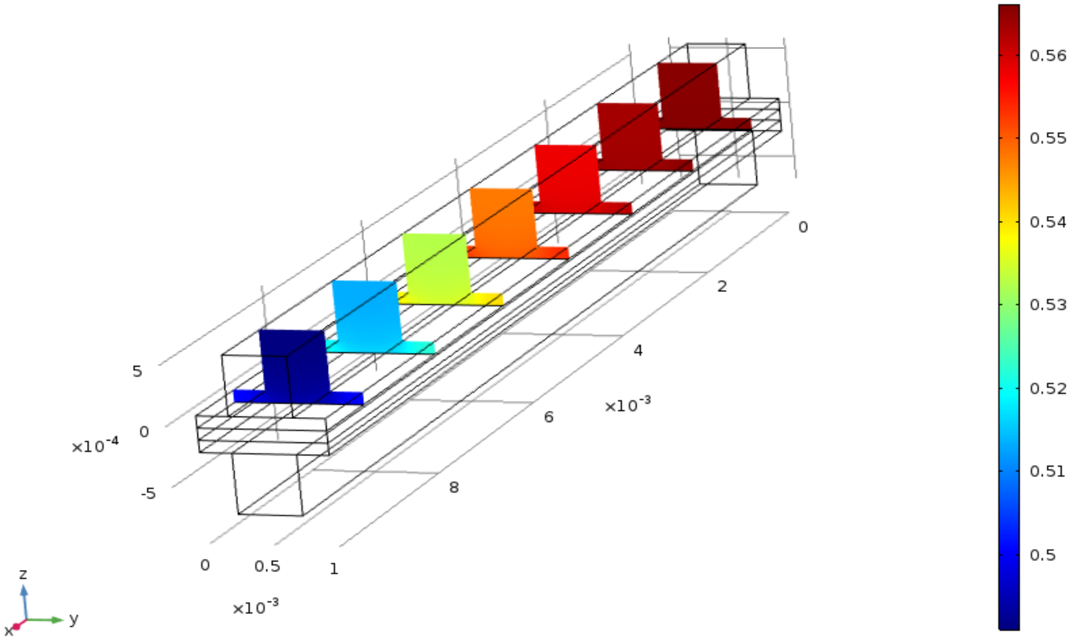


Figure 37: Mass fraction of nitrogen at cathode

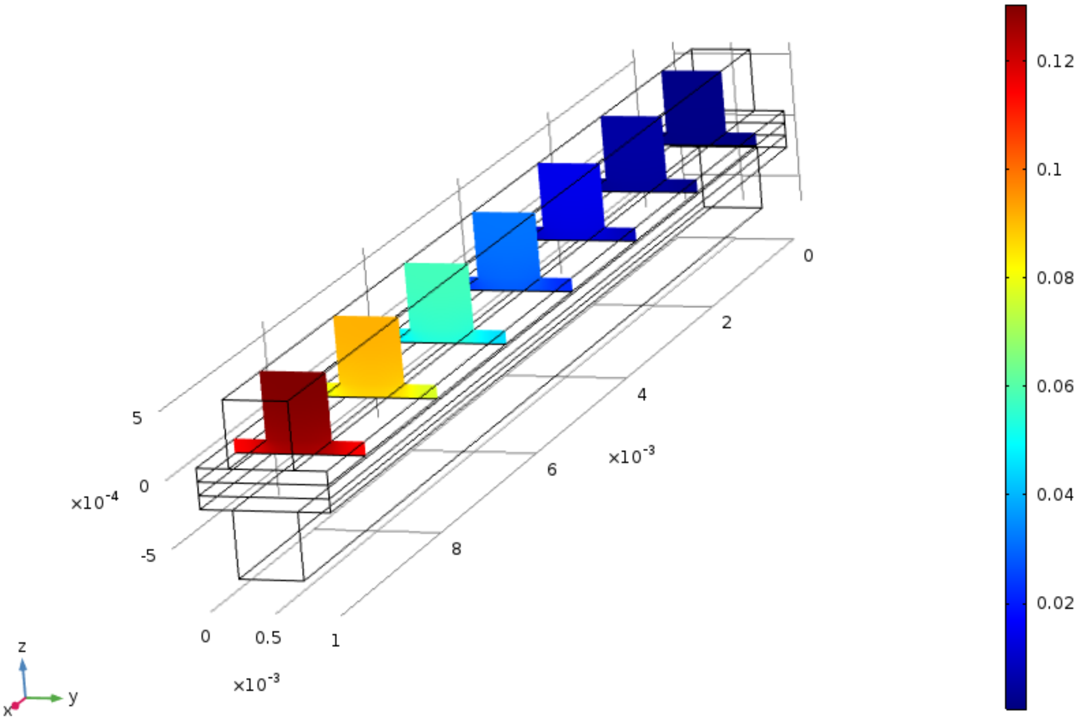
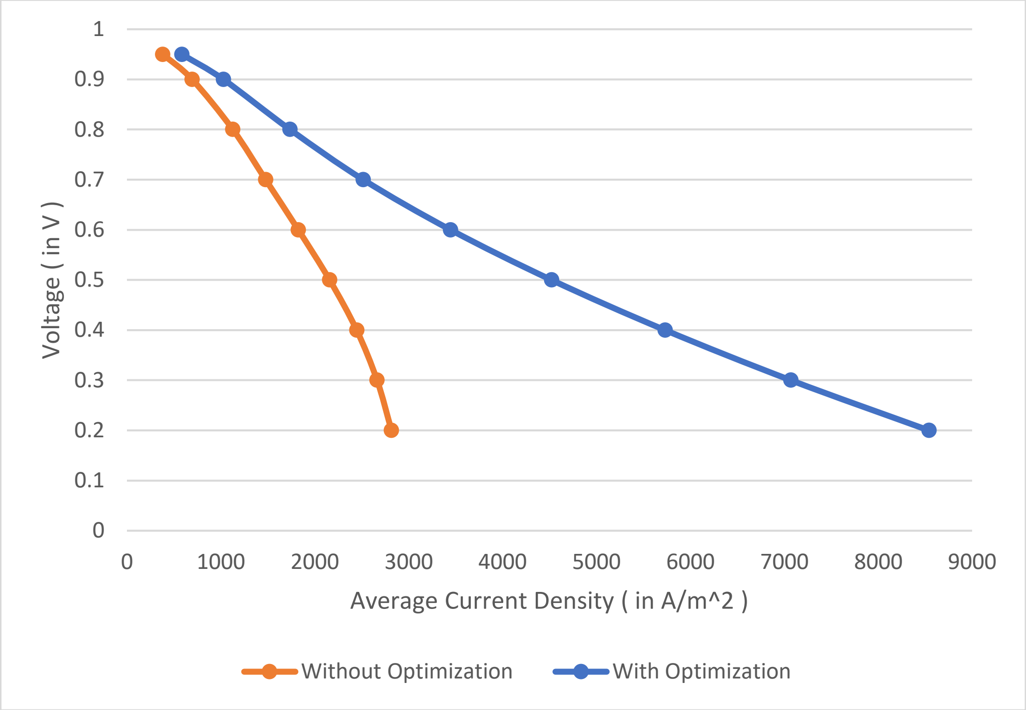


Figure 38: Mass fraction of oxygen at cathode

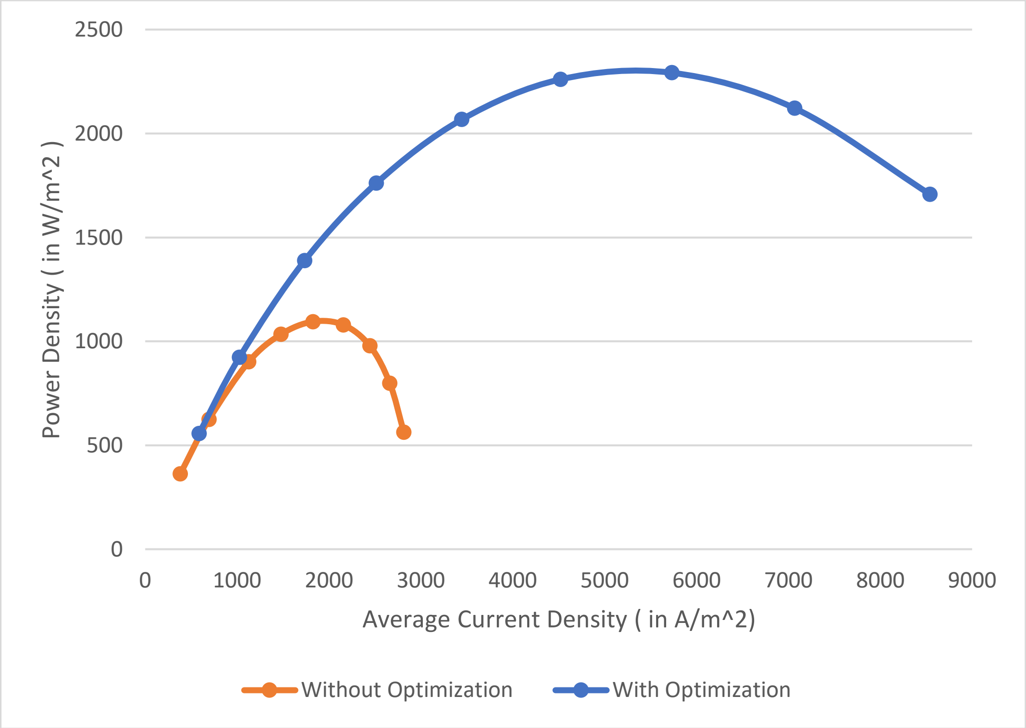
5.9.7 Combined effect of all the parameters:



Normal Parameters

- Temperature=800 Degree Celsius
- Atmospheric Pressure = 1 atm
- Electrolyte Porosity = 40 %
- Electrolyte Thickness =100 microns
- Cell Length = Full cell length of 10 mm

Figure 39: Optimized parameters impact on polarization curve



Optimum Parameters

- Temperature=600 Degree Celsius
- Atmospheric Pressure = 5 atm
- Electrolyte Porosity = 40 %
- Electrolyte Thickness =15 microns
- Cell Length = Half cell length of 5 mm

Figure 40: Optimized parameters impact on power density

CHAPTER 6

Modeling and Simulation of SOEC using COMSOL Water Electrolyzer Module

6.1 Introduction

- A solid oxide electrolyzer cell (SOEC) is a type of solid oxide fuel cell (SOFC) that operates in a regenerative mode. It utilizes a solid oxide or ceramic electrolyte to electrolyze water or carbon dioxide, producing hydrogen gas or carbon monoxide and oxygen.
- SOECs have the advantage of producing pure hydrogen, which is a clean fuel that can be stored and utilized as an alternative to batteries, methane, and other energy sources. This makes them attractive for various applications that require clean and efficient energy conversion and storage systems.[37]
- Solid oxide electrochemical cells, particularly solid oxide electrolysis cells, hold significant promise as energy storage devices. These cells utilize surplus electrical energy, often from renewable sources, to drive electrochemical reactions and produce fuels containing chemical energy, such as methane or diesel. These fuels can then be utilized within existing fuel infrastructure.
- Solid oxide electrolysis cells are often described as the reversible operation of fuel cells. While fuel cells generate electricity from fuels, electrolysis cells produce fuels to store electricity. In essence, electrolysis cells can be thought of as batteries, where instead of storing electrical energy in metals as traditional batteries do, they store electricity in the form of fuels like hydrogen and carbon monoxide. This enables the storage of electrical energy in a chemical form, providing potential solutions for energy storage and distribution.[38]

6.2 Model Assumptions:

- Surface-to-surface radiation between internal boundaries is neglected
- Constant conductivity is assumed throughout the electrolyte
- Model considers high electrical conduction between electrodes
- Electrochemical reactions happening at the triple phase boundary only
- High rate of Ionic conduction is considered in the electrolyte along with very low electrical conduction
- Mass transport phenomenon is dominating in porous electrodes
- Only O2 and N2 are considered in Anode flow channel as air (rest gases are neglected for simplification

6.3 Model Description:

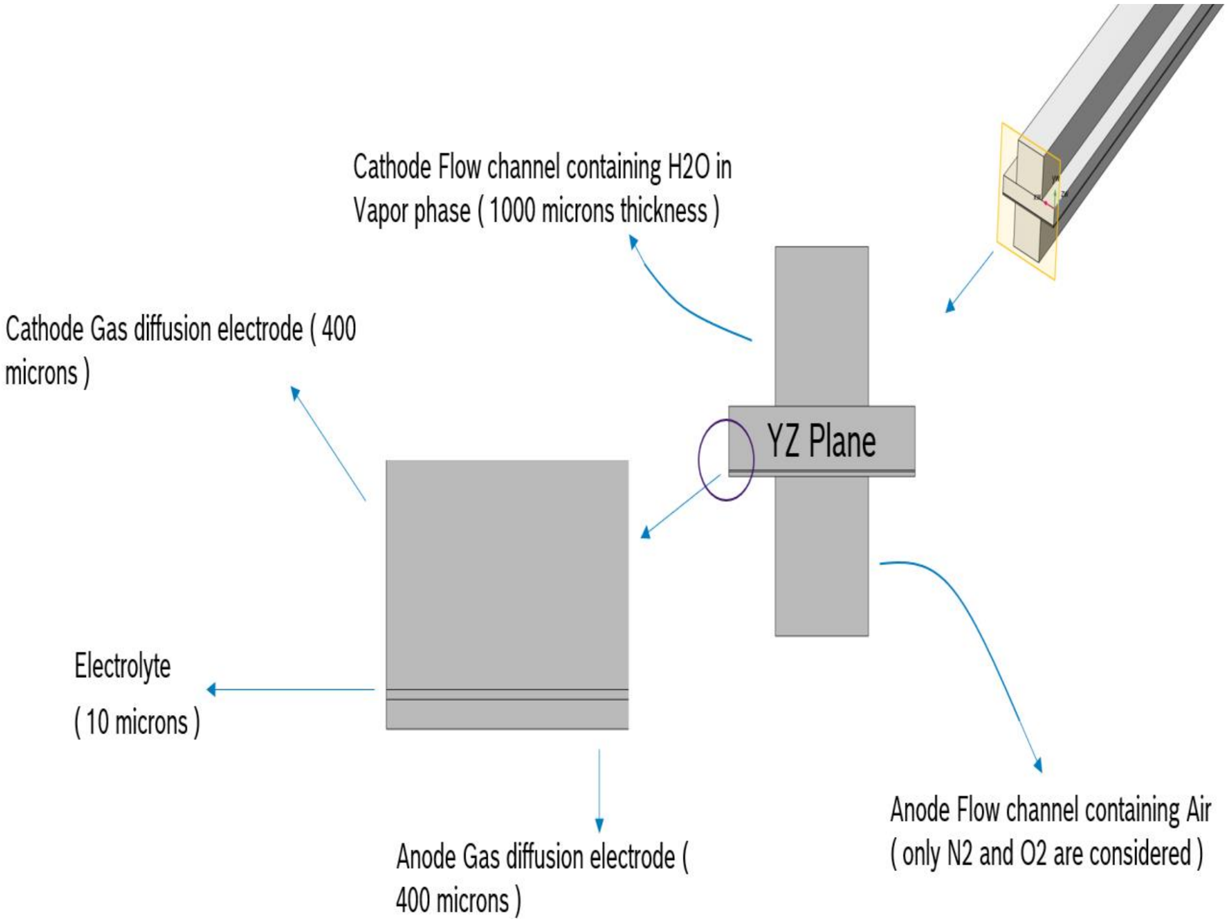


Figure 41: SOEC model description

There are basically 3 ways by which we can model SOEC in COMSOL Multiphysics. Those are described below:

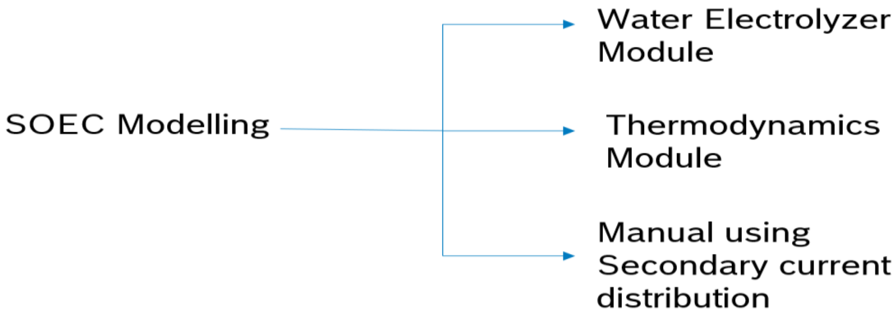


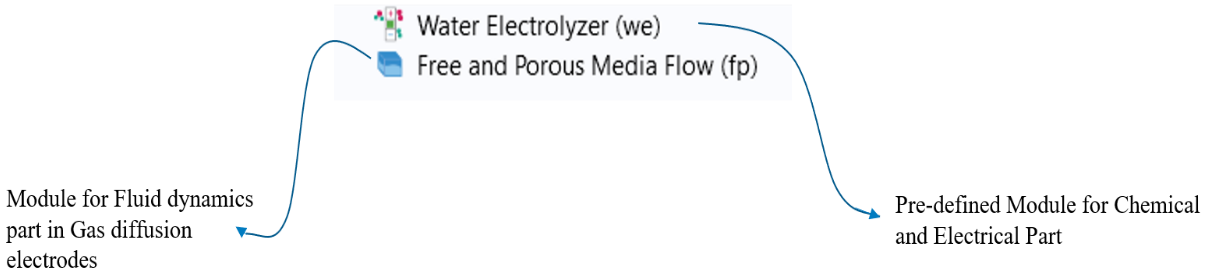
Figure 42: Various approaches to electrochemical modeling

On the anode, oxygen ions are oxidized to form oxygen gas, whereas on the cathode, water vapor is reduced to form hydrogen gas and oxygen ions[39]

Water Electrolyzer Module- This module interface is used to define the electrode reactions and the electrolyte charge transport in the porous gas diffusion electrodes and the electrolyte layer, as well as the mass transport of hydrogen and water.

The momentum flow is defined in the model using the Free and Porous Media Flow interface. Brinkman equations are used for the porous gas diffusion electrodes and Navier-Stokes equations

The properties of the cathode gas mixture, as well as the equilibrium potentials of the electrode reactions are automatically defined by the default built-in options of the Water Electrolyzer interface[39]

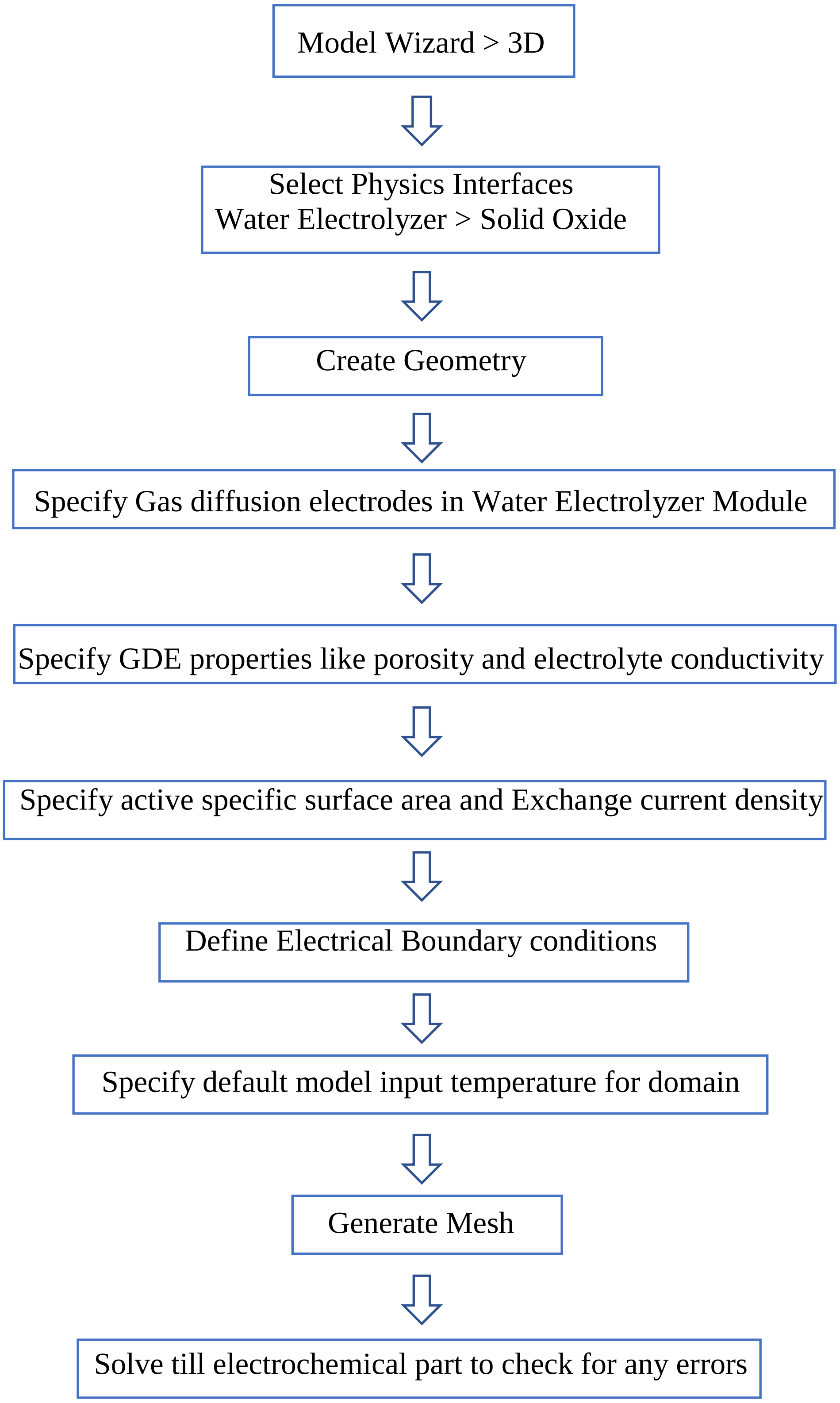


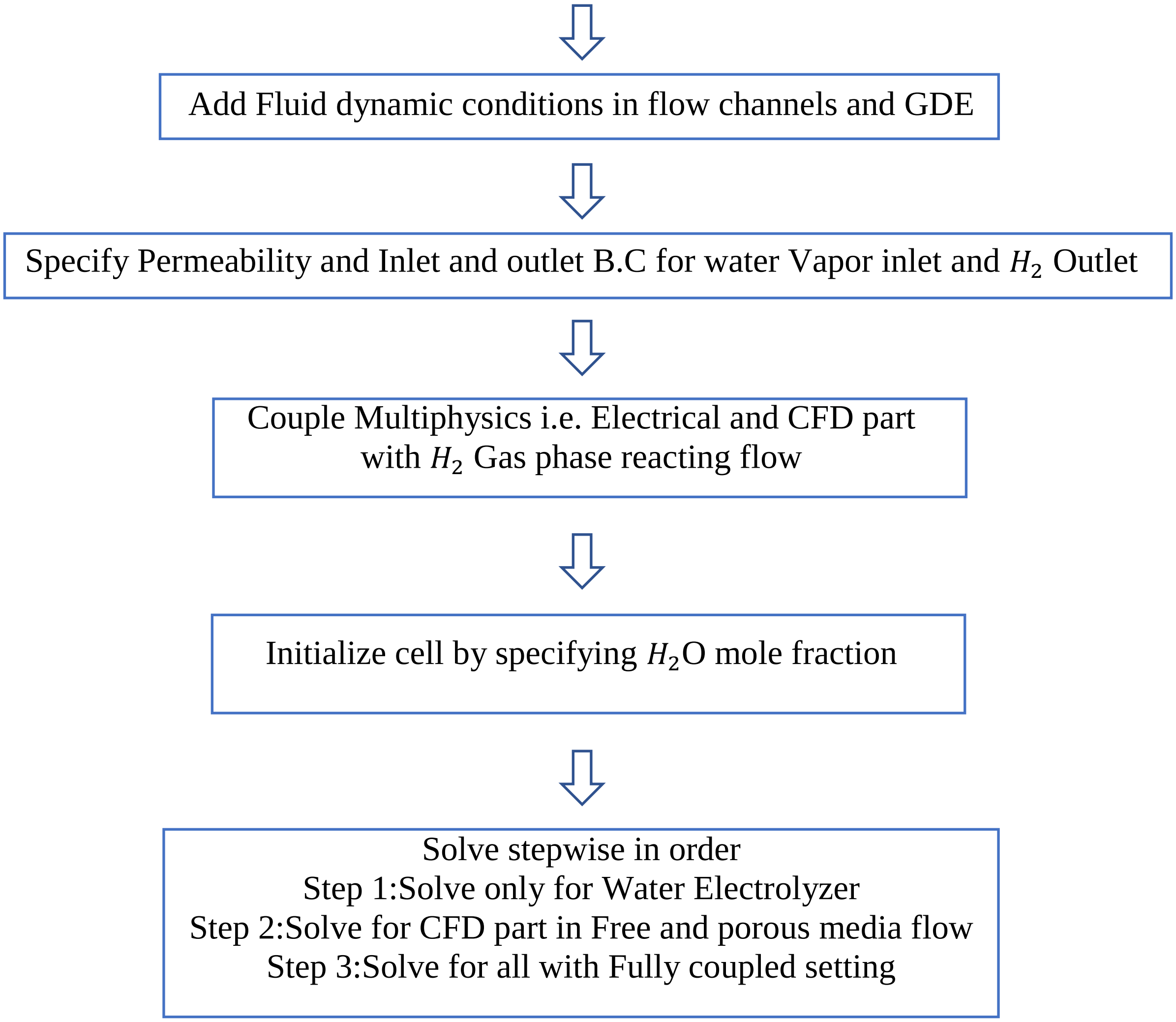
6.3.1 Geometrical Parameters:

Table 5: Dimensional parameters used for SOEC

Cell width	2.0×10^3	µm
Cell Length	4.0×10^4	µm
Rib thickness	500	µm
Fuel/airchannel width	1.0×10^4	µm
Electrolyte thickness	10	µm
Hydrogen electrode thickness	400	µm
Oxygen electrode thickness	30	µm
Fuel/air channel thickness	1.0×10^3	µm
Interconnect thickness	300	µm

6.4 Methodology





Add Fluid dynamic conditions in flow channels and GDE

Specify Permeability and Inlet and outlet B.C for water Vapor inlet and H_2 Outlet

Couple Multiphysics i.e. Electrical and CFD part with H_2 Gas phase reacting flow

Initialize cell by specifying H_2O mole fraction

Solve stepwise in order
Step 1:Solve only for Water Electrolyzer
Step 2:Solve for CFD part in Free and porous media flow
Step 3:Solve for all with Fully coupled setting

6.5 Boundary Conditions:

Property	**Values**	**Units**
Reference (inlet) temperature	800	◦C
Reference (outlet) pressure	1	atm
Specific surface area, H_2electrode	1.3×10^6	1/m
Specific surface area, O2 electrode	1.075×10^6	1/m
Permeability, hydrogen electrode	1.0×10^{-10}	m^2
Permeability, oxygen electrode	1.0×10^{-10}	m^2
Reference diffusivity	3.16×10^{-8}	m^2/s
Pressure drop, Hydrogen electrode	150	Pa
Pressure drop, oxygen electrode	800	Pa

Table 6 : Physics parameters used in SOEC study

- Material used was Yttria Stabilized Zirconia for the solid electrolyte and its properties were taken by default from COMSOL material library database.
- Yttria is added to stabilize the conductive cubic fluorite phase, as well as to increase the concentration of oxygen vacancies, and thus increase the ionic conductivity[40]

6.5.1 Electrical Boundary Conditions:

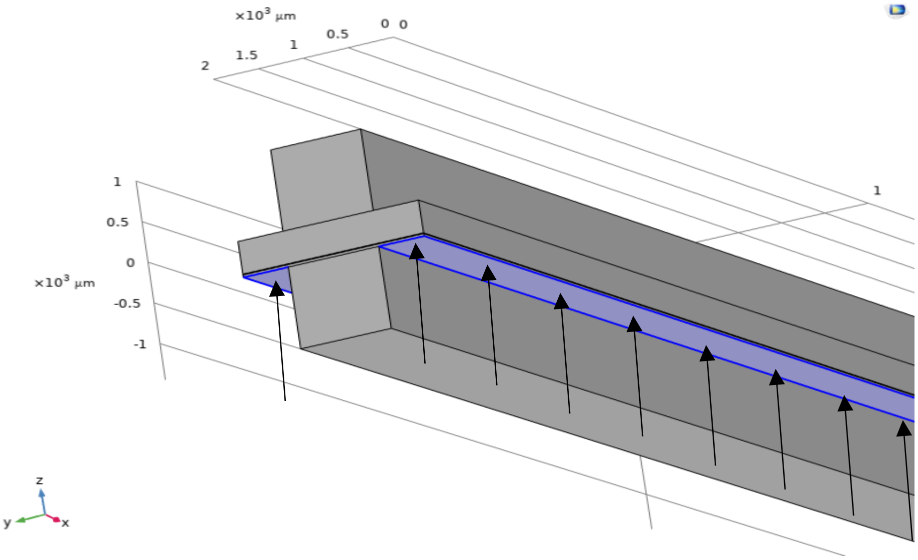


Figure 43: Electrode current boundary condition; SOEC

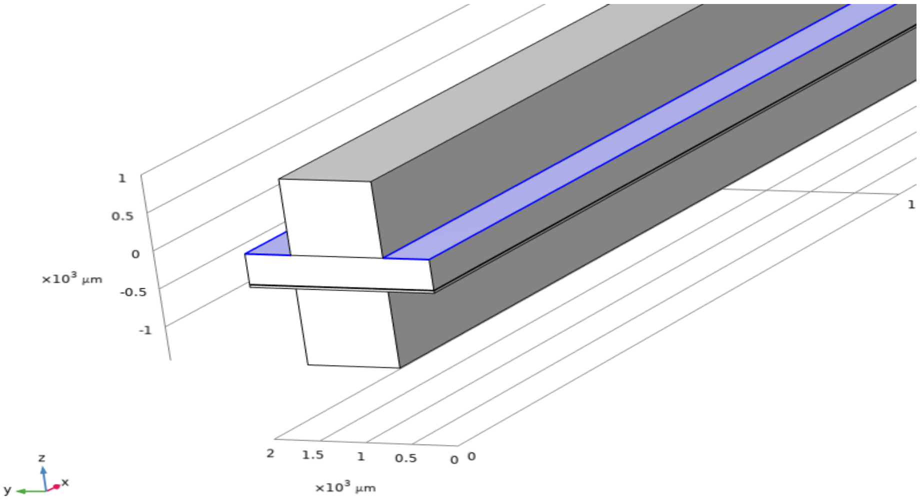


Figure 44: Electric ground condition at cathode GDE

- An Inward Electrode current of 10,000 A/m^2 was applied on the Anode side of SOEC (or air electrode in general).

- An Electric ground condition is also applied on the top of cathode Gas diffusion electrode to ensure the flow of current should happen from Anode to cathode in case of SOEC
- An electric potential of 1 Volts was considered at the bottom of Anode GDE along with current condition.
- ECD at cathode gas diffusion electrode is considered as 0.1 [A/m^2] and at the anode as 0.01 [A/m^2]
- Effective electrical conductivity at hydrogen electrode i.e. Cathode GDE and anode GDE was taken as 465 S/m
- Electrolyte conductivity of 5 S/m was considered.

6.5.2 CFD and chemistry boundary conditions:

- Inlet mole fraction at cathode inlet was taken as 0.5 and for O2 as 0.21
- The porosity was taken as 40 % for both cathode GDE and Anode GDE
- The pressure drop condition of 150 Pa is applied on the inlet of Cathode where steam is fed and for anode GDE the condition was 800 Pa is considered
- The inlet steam stoichiometry was taken as 1.1
- Electrode permeability of 1e-10[m^2] was considered for Cathode and anode gas diffusion electrodes
- The charge transfer coefficient of 0.5 was taken in the butler-Volmer expression

6.6 Meshing Approach

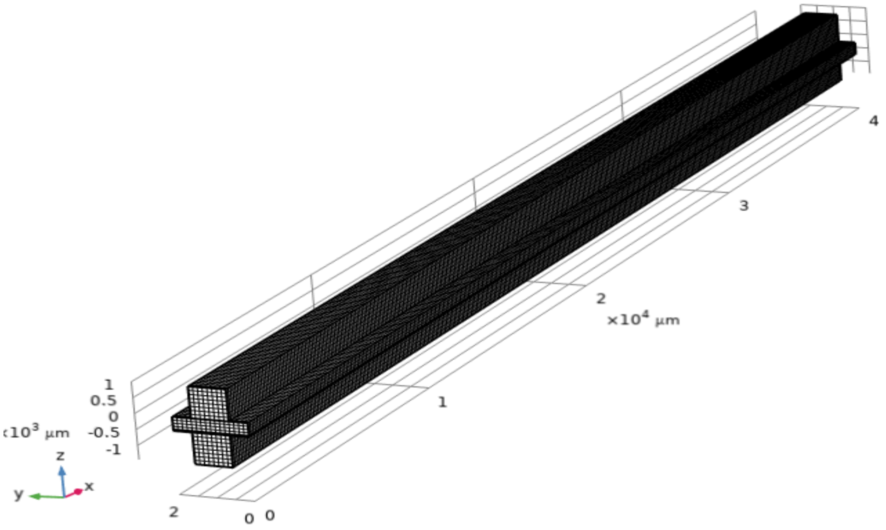


Figure 45: SOEC meshing

- A mapped mesh of hexahedral nature was considered for this study.
- The maximum element size of 125 microns was used and minimum was 62 microns
- 8 Boundary layers with a stretching factor of 1.2 were considered in the areas near to the

gas diffusion electrodes

- Complete mesh consists of 71680 domain elements, 40128 boundary elements, and 5368 edge elements

6.7 Results and Discussion:

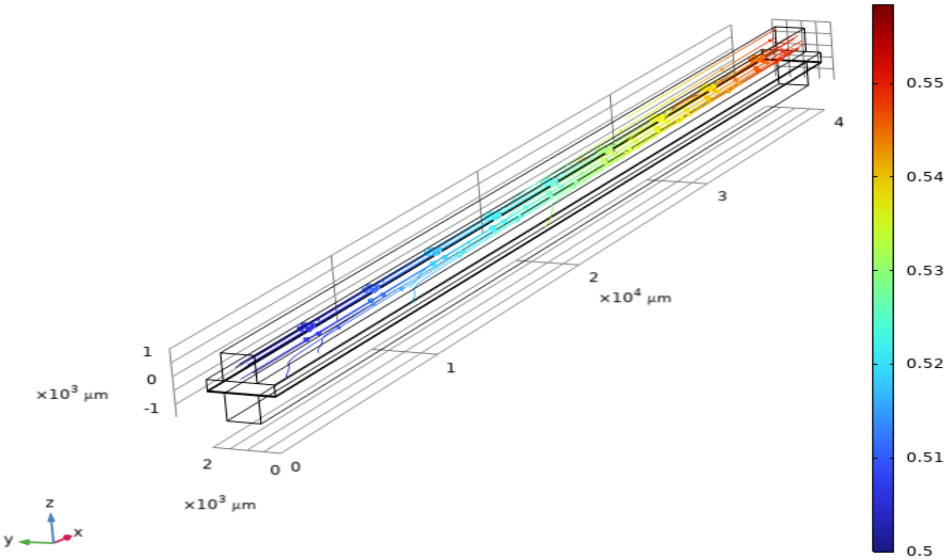


Figure 46: Mole fraction streamline of hydrogen gas production at cathode

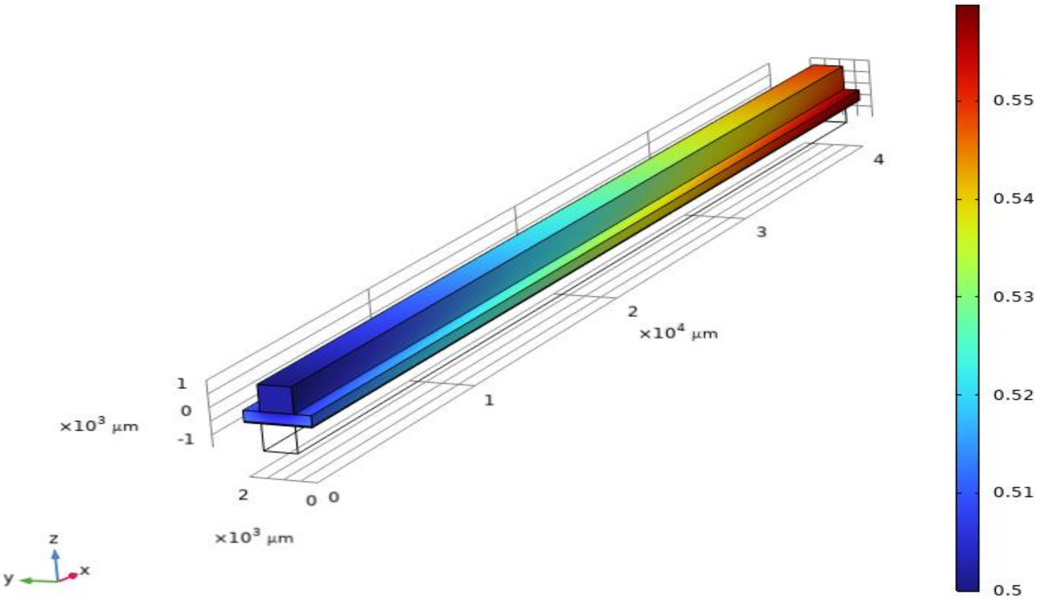


Figure 47: Mole fraction of hydrogen gas at surface

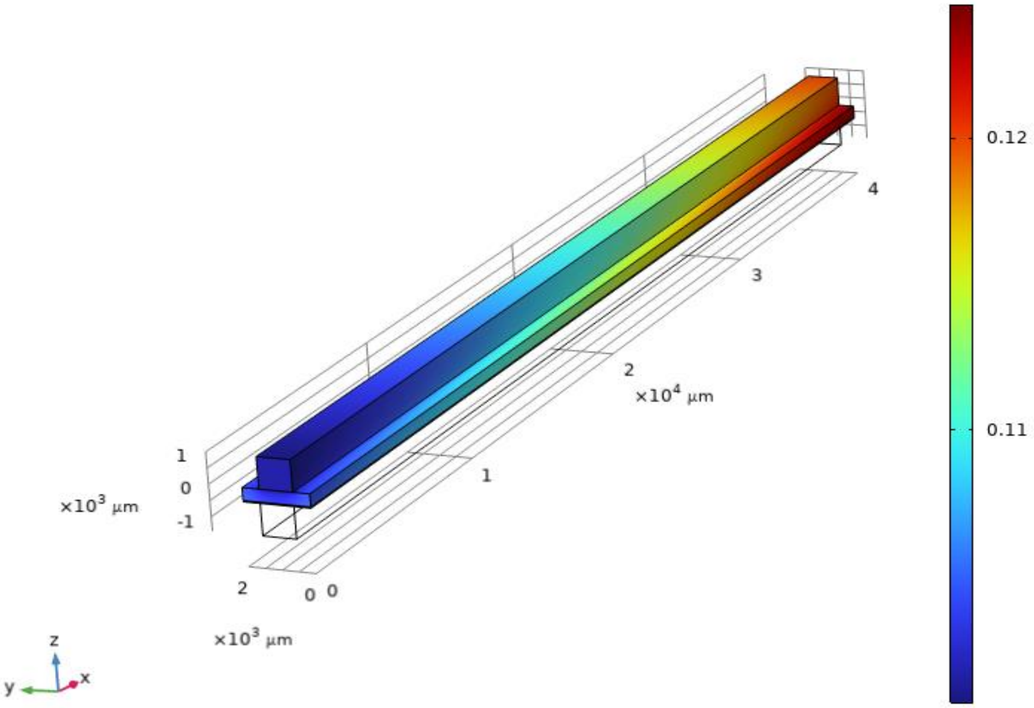


Figure 48: Mass fraction of hydrogen gas at cathode

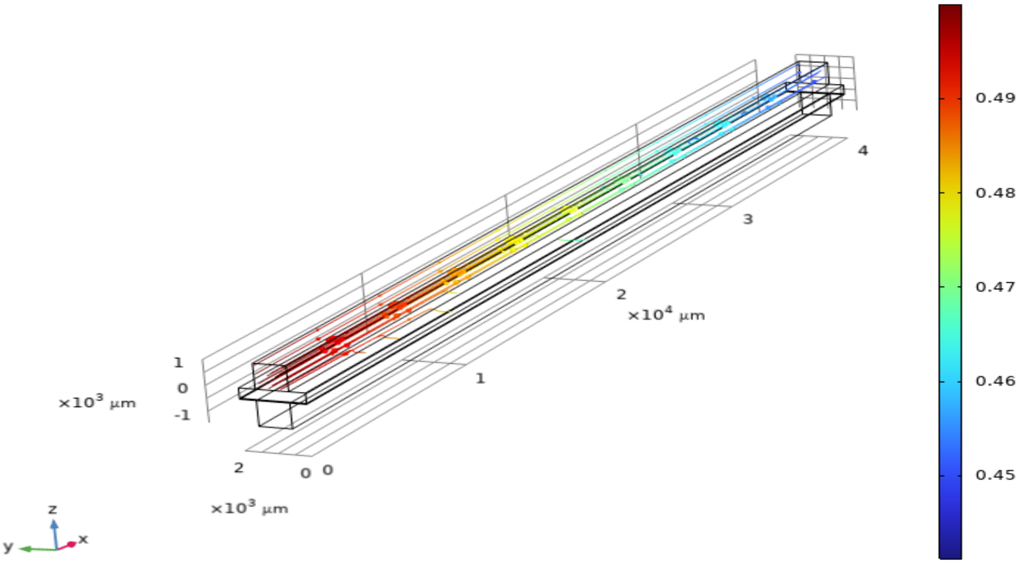


Figure 49: Mole fraction streamline of water consumption along length

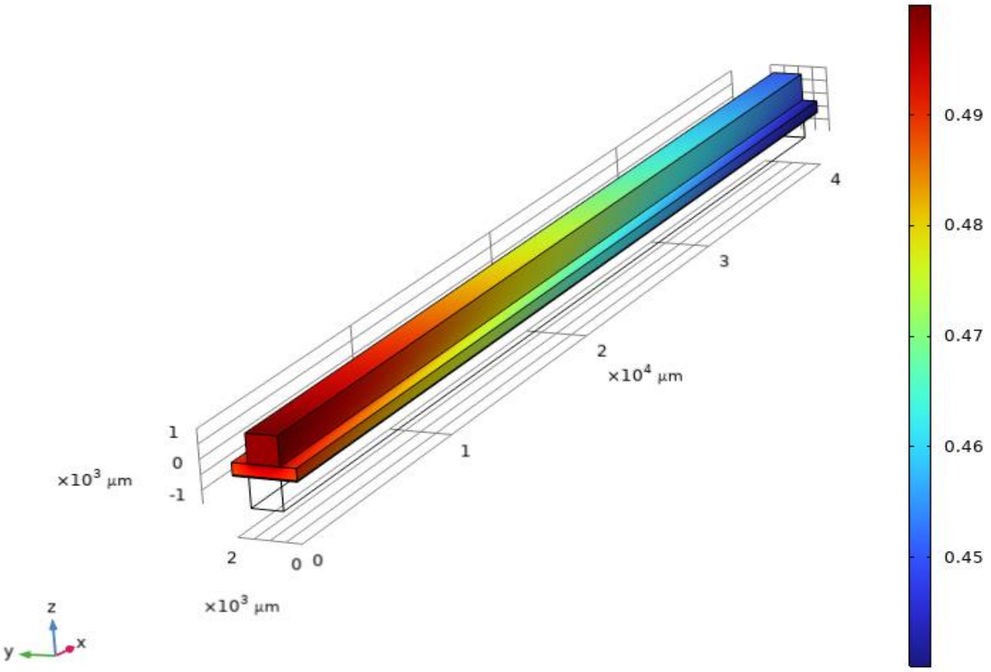


Figure 50: Mole fraction of H_2o at surface

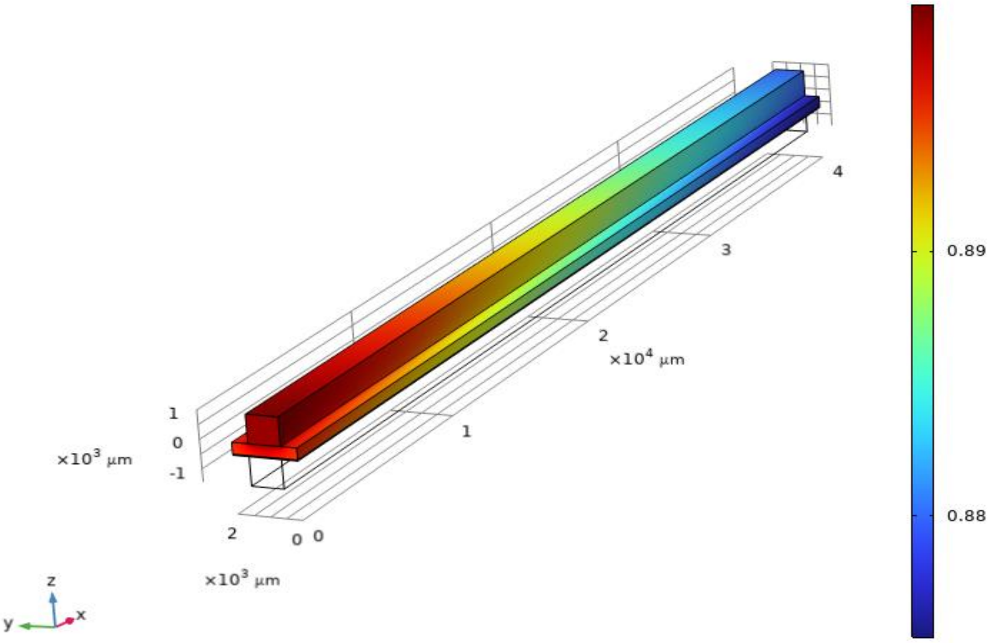


Figure 51: Mass fraction of H_2o at surface

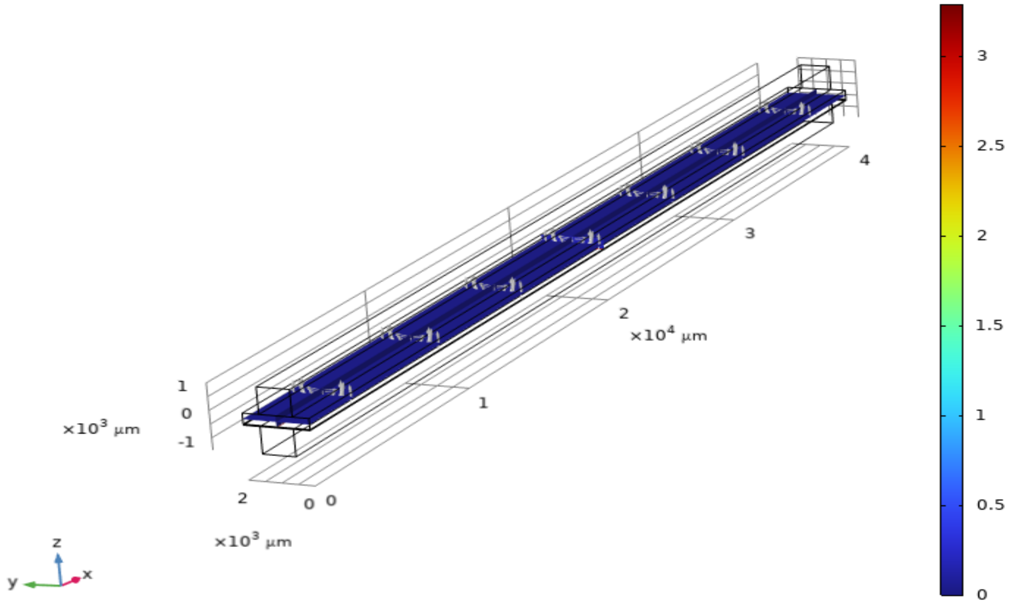


Figure 52: Electrode potential with respect to ground

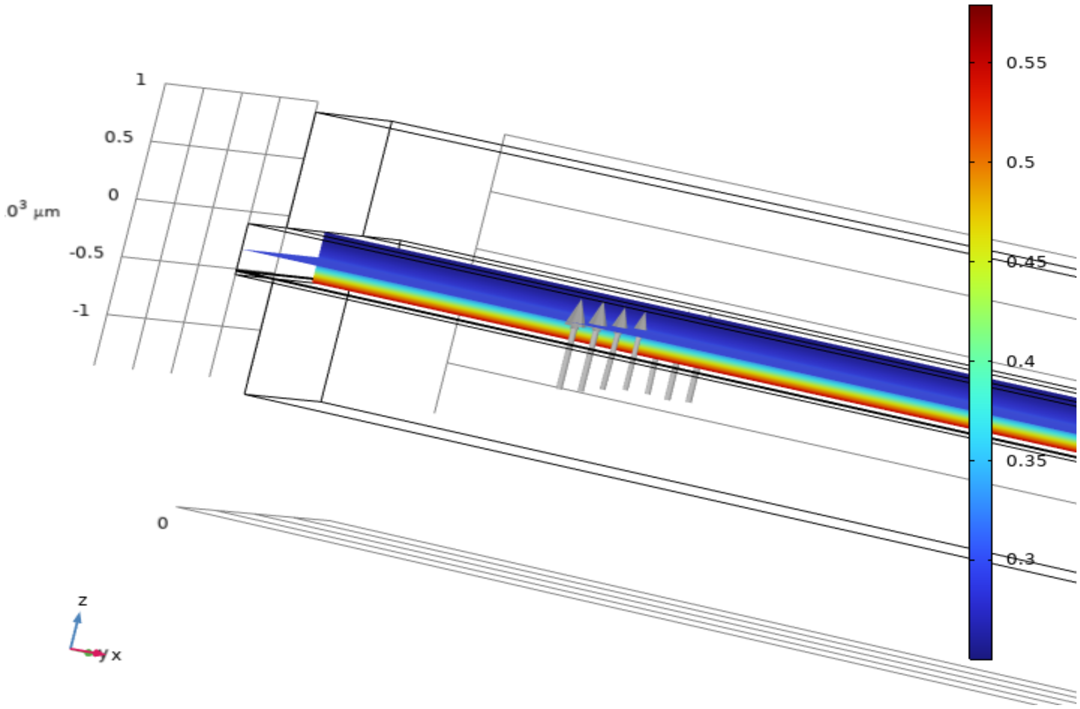


Figure 53: Electrolyte potential

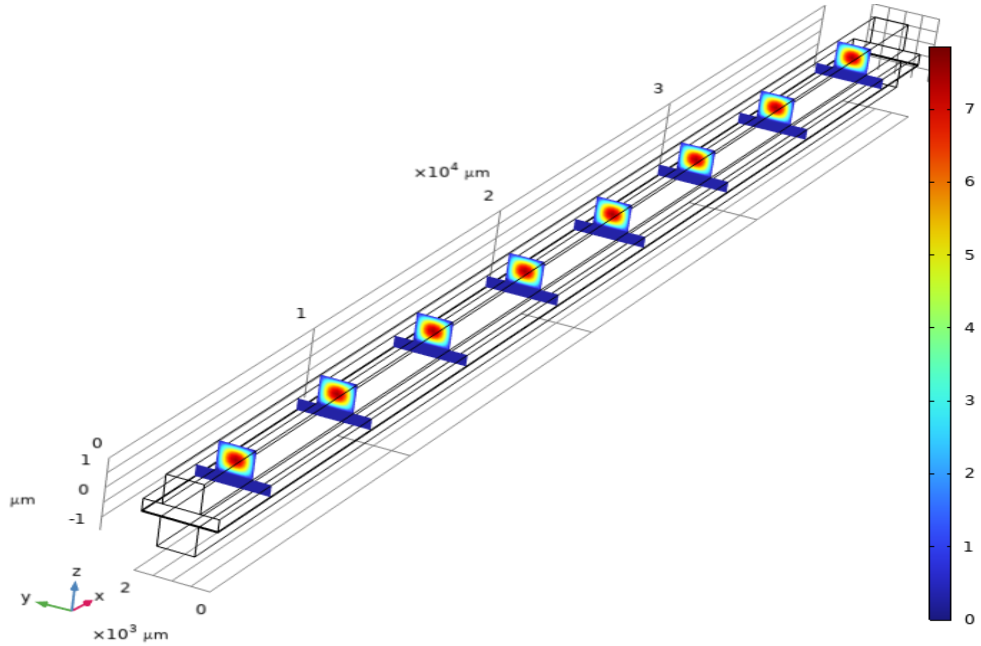


Figure 54: Velocity slice at cathode flow channel and GDE

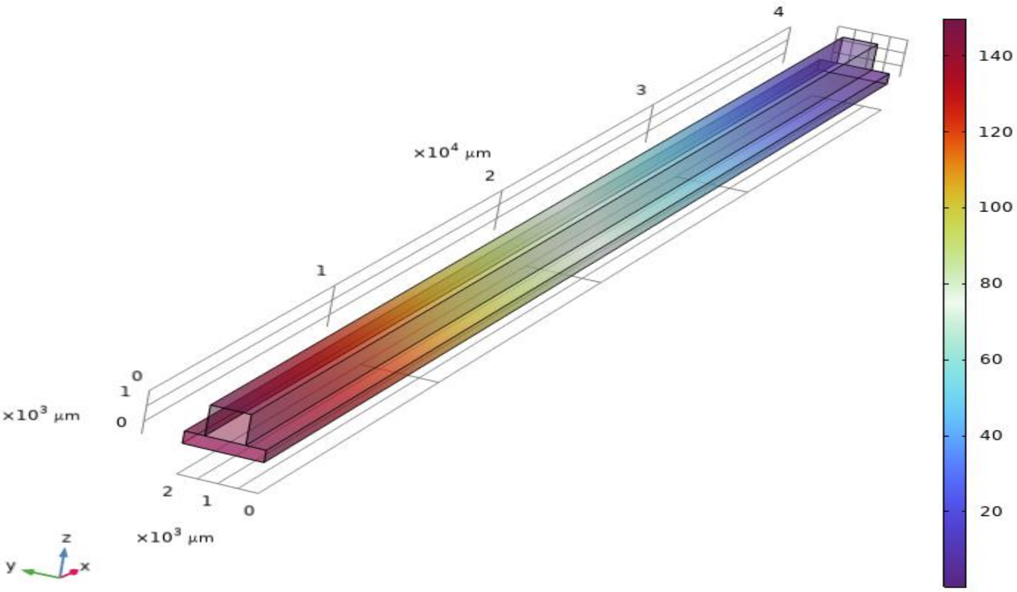


Figure 55: Pressure distribution at cathode flow channel and GDE

Chapter 7

Conclusion and Future Scope

7.1 Conclusion

From this project we can conclude that by varying some parameters either in SOFC or in SOEC, there is a huge role in obtaining the maximum output from the system. As we have seen in previous pages that the peak power density is almost doubled when the length is reduced to its half, and average current density is almost thrice its value by using all parameters effect combined.

Also, this thesis discussed the impact of pressure, temperature, electrode porosity, electrolyte thickness, cell length and then also considered simultaneous impact of all of those parameters combined. So, in conclusion this M.Tech Thesis will help anyone who wants to know about fuel cell in detail and what are the most important parameters for the study

Also, one thing to note that this study is based on simulation parameters and in reality we have to consider constraints on some of the parameters for safety and efficiency concerns due to some practical limitations.

7.2 Future Scope

- Evaluation the impact of input parameters on hydrogen production in solid oxide electrolysis cell
- Exploring optimized process techniques to approach the problem
- To develop a reversible model which can work in both SOFC and SOEC mode
- Impact of using pure oxygen on cathode side instead of Air
- Finding out Efficiency of the cell and parameters that will impact it
- Developing a method for finding out at what temperature, reactions will start to take place
- Impact of material properties like Electrolyte conductivity, Solid effective conductivities & permeability on Performance parameters

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