Numerical simulation of Proton Exchange Membrane Fuel Cell using COMSOL Multiphysics and elucidating the effect of different flow rates and temperatures

Dr Mishma S Stanislaus[1], Dr Lathapriya V[1], Dr Anand M Shivapuji[2], Prof S Dasappa[3]
[1] Research Scientist; [2] Senior Research Scientist; [3] Professor and Chair
Interdisciplinary Center for Energy Research, Indian Institute of Science; Bangalore, KA-560012, India

Abstract

In this study, COMSOL Multiphysics is employed to develop a comprehensive numerical PEMFC model with a primary focus on investigating the effects of different anode and cathode fuel flow rates across a specific temperature range on the PEMFC's performance characteristics. The developed PEMFC model considers a three-dimensional domain, accounting for the anode flow channel, anode, the proton exchange membrane, cathode and cathode flow channel. Further, simulated PEMFC model integrates Multiphysics phenomena, including mass transport, momentum transport, electrochemical reactions, and fluid dynamics, to capture the complex interactions within the PEM fuel cell structure. The electrochemical reactions are represented using appropriate kinetics (Butler-Volmer) and thermodynamics, while transport phenomena are described using Maxwell-Stefan diffusion and convection equations. Likewise, the flow distribution of the PEMFC model is addressed using Navier-Stokes and Brinkmann equations. The model's accuracy is validated against experimental data. To explore the effects of fuel flow rates, a parametric study is conducted, encompassing a wide spectrum of operating temperatures of 30- 90 ^{o} C. The fuel flow rates are systematically adjusted (H_2:O_2 → 100:100, 100:200, 200:100 and 200:200) while monitoring key performance metrics such as cell voltage, current density, power density and overall efficiency. From the polarization and power curves, it is observed that as the temperature increases, the current density and power density values are decreasing gradually at all the fuel flow rates employed. The maximum current density and power values obtained at an optimized fuel flow rates of H_2:O_2 (200:100) are 61049 A/m^2 and 13966 W/m^2 at 30 ^{o} C. The difference in the current and power density values observed while varying fuel flow rates is due to fuel starvation or flooding which limits reactants transportation. The decrease in the current and power density with increasing temperature is due to the low concentration of H_2O (0.001 mol%) employed in the model. Due to dry conditions inside the cell, the proton conduction inside the model is hindered, which in turn limits the current density. The distribution of reactants within the cell in accordance with varying fuel flow rates that affects the electrochemical reactions is also analyzed, in order to understand the performance of PEMFC. This study provides valuable guidance for optimizing PEMFC operation under varying temperature and fuel flow rate conditions. The developed COMSOL model serves as a versatile platform for further investigations into novel designs and advanced operating strategies.

Keywords: Proton Exchange membrane Fuel cell, Green Hydrogen, Fuel flow rates, Performance optimization

Introduction

Proton Exchange Membrane Fuel Cells (PEMFCs) represent a promising and sustainable technology for clean energy conversion, offering high energy efficiency and minimal environmental impact [1]. They have garnered significant attention in recent years due to their potential applications in various sectors, including automotive, stationary power generation, and portable electronics [1]. However, the efficient and reliable operation of PEMFCs remains a complex challenge influenced by several interconnected parameters such as operating temperature, pressure, humidity and fuel flow rates.

Among these, flow rates and operating temperatures are crucial factors that significantly affect the durability and cell performance. Further, controlling the flow rates of reactant gases and maintaining suitable operating temperatures are critical to ensuring efficient proton transport and preventing issues such as flooding or drying out of the membrane, which can deteriorate cell performance. Hence, to optimize the design and operation of PEMFCs for practical applications, it is imperative to gain a deep understanding of how different flow rates and temperatures impact their performance and efficiency [2]. Additionally, addressing the reliability and durability issues of

PEMFCs is also essential for their widespread adoption. Therefore, there is a pressing need for comprehensive research that investigates the intricate interplay between flow rates, temperatures, and PEMFC behavior [3]. Numerical modelling and simulation of PEMFCs plays a pivotal role in optimizing their design, operation, performance and understanding their complex behavior. COMSOL Multiphysics, a versatile finite element analysis software, provides an ideal platform for simulating complex Multiphysics phenomena like those encountered in PEMFCs. Its ability to couple various physics domains, including fluid flow, heat transfer, and electrochemistry, makes it a powerful tool for investigating the interdependencies between flow rates and temperatures in a PEMFC. The software allows researchers to build accurate computational models that replicate real-world conditions and provides insights into phenomena that are challenging to study experimentally [4].

However, there is a noticeable research gap in terms of a comprehensive analysis that considers the simultaneous influence of both parameters. Such a study is crucial because real-world PEMFC applications involve dynamic changes in operating conditions, making it vital to understand their combined effects. In addition, Hydrogen is used to operate a single-cell PEMFC, and the obtained experimental data is compared with the simulated models. Hence, herein, in the present study we constructed a PEMFC model using COMSOL Multiphysics and investigated the effect of fuel flow rates (anode/cathode) over a wide span of temperature range of 303.15 K-363.15 K. Further, the distribution of concentrated species, fluid flow and electrochemical performance of the modelled PEMFC is studied and the model is validated by comparing with experimental results of UHP-Hydrogen operated fuel cell.

Methodology

Experimental method

The assessment of high-temperature proton exchange membrane fuel cell (HT-PEMFC) performance was conducted utilizing the Magnum H&H-Gmbh FC Midi test bench, capable of handling up to 5 V voltage and 150 A current. To investigate the fuel cell's performance, the following steps were taken:

Initially, the fuel cell assembly, which included the membrane electrode assembly (comprising the anode, Nafion membrane, and cathode), anode/cathode flow channels, bipolar plates, current collectors, and end plates, was meticulously put together. MEA with membrane active area of 5cm^2 was used for all experiments. This assembly was then connected to the test station, and the open circuit voltage (OCV) was duly recorded. Following an hour-long conditioning period at 2A, a polarization and power curve was established under constant current conditions serving as the baseline.

Figure 1. Photograph of the HT-PEM Fuel cell test bench, Fuel cell assembly and the Membrane Electrode Assembly used in the present work.

Table 1. Experimental & Simulated Fuel Feed (mL/min)

Case	I	II	III	IV
Hydrogen (H_2)	100	100	200	200
Oxygen (O_2)	100	200	100	200

Subsequently, additional polarization and power curves were generated under varying conditions, specifically by altering fuel flow rates (as outlined in Table 1) and adjusting temperatures. The entire assembly, along with the test station, is visually depicted in Figure 1 for reference.

PEMFC Modelling Methods and Details

COMOSL Multiphysics version 6.0 is employed to develop comprehensive numerical PEM fuel cell model. This PEMFC model is designed to be highly inclusive, considering a three-dimensional (3D) domain that encompasses the various components, including the anode flow channel, anode Gas Diffusion Electrode (GDE), the proton exchange membrane (Nafion), cathode GDE, and cathode flow channel (Figure 2). For the sake of clarity, the dimensions of the modeled PEMFC and the specific cell parameters employed for studying the cell's performance are detailed in Tables 2 and 3.

All other definitions and equations used were manually entered into the model as prescribed variables. To simulate the PEMFC model, we first design the 2D layout of the components. Subsequently, we extend this design into a 3D domain for in-depth analysis. The performance of the fuel cell, the distribution of species concentrations, velocity profiles, pressure distribution, and electrochemical behavior of the PEMFC model are comprehensively evaluated using predefined modules and physics. These include the

Hydrogen fuel cell module and the Free and Porous Media Flow module.

Table 2. Cell dimensions of simulated PEMFC model

Cell Dimensions	
Cathode Flow channel Width	1.5 mm
Cathode Flow channel Height	0.2 mm
Anode Flow channel Width	1.5 mm
Anode Flow channel Height	0.2 mm
Anode Gas Diffusion Electrode thickness	130 µm
Cathode Gas Diffusion Electrode thickness	130 µm
Electrolyte/Membrane thickness	30 µm
Rib width	1.0 mm

Table 3. Cell parameters used to study the performance of simulated PEMFC model

Cell Parameters	
Pressure	1 atm.
Temperature	303.15-363.15 K
GDL permeability	1.18E-11 m²
Permeability (porous electrode)	2.36E-12 m²
GDL electric conductivity	222 S/m
Membrane Conductivity	9.825 S/m
Exchange current density, anode	0.1 A/m²
Exchange current density, Cathode	0.01 A/m²
Porosity	0.4

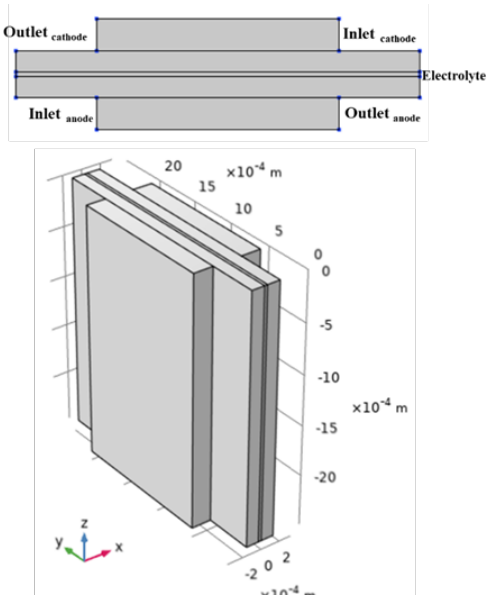

Figure 2. Geometry of PEMFC model constructed using COMSOL Multiphysics in 2D and 3D domains

The model is composed of five distinct domains, featuring 30 faces and 56 edges. The mesh for this model consists of 1704 elements, each with a minimum element quality of 0.8293 (Figure 3).

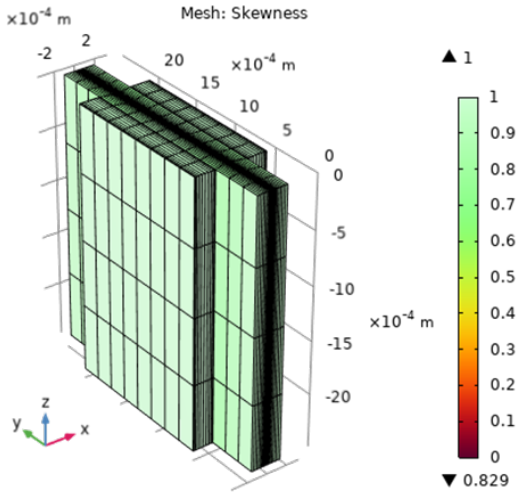

Figure 3. Mesh quality distribution of PEMFC Model

In order to solve the current model, we adopted a segmented step-by-step approach, utilizing the PARDISO solver with an overarching relative tolerance set at 0.001. The sequence of these segmented steps followed this sequence:

- Addressing electronic and ionic potentials
- Solving for velocity and pressure
- Managing the distribution of cathode and anode species
- Regulating temperature and measuring polarization and power curves at different temperatures.

For the purpose of generating polarization curves, we executed a parametric voltage stepping procedure, with increments of 0.05, spanning from 0.95 V to 0.1 V.

The main focus of the present study lies in the exploration of how varying anode and cathode fuel flow rates, within a defined temperature range, impact the performance attributes of the PEMFC (Table 1). To ensure the accuracy of this model, it is rigorously validated against experimental data, thereby confirming its reliability in simulating the behavior and performance of PEMFCs.

Governing Equations

The constructed three-dimensional PEMFC model comprises various components, including the anode flow channel, anode Gas Diffusion Electrode (GDE), the proton exchange membrane, cathode GDE, and cathode flow channel. This model is designed to encompass a multitude of physical phenomena, such as mass transport, momentum transfer, electrochemical reactions, and fluid dynamics, in order to capture the intricate

interactions occurring within the structure of the PEM fuel cell. In this model, the electrochemical reactions are mathematically represented using appropriate charge transfer kinetics, specifically the Butler-Volmer equation, and are thermodynamically consistent. Furthermore, the transport processes are described utilizing the Maxwell-Stefan diffusion equations and convection equations, which account for the complex movement of various species within the fuel cell. Simultaneously, the distribution of fluid flow within the PEMFC model is comprehensively addressed through the incorporation of the continuity, Navier-Stokes equations (anode & cathode flow fields) and the Brinkmann equations (porous electrodes), which take into consideration the intricate fluid dynamics within the fuel cell structure.

The boundary conditions entail the requirement of zero velocity gradients (i.e., no-slip conditions) along the walls, and the need to set prescribed inlet velocities, pressure drop at both the anode and cathode.

Results and Discussion

Figure 4 illustrates the distribution of electrolyte potential and electrolyte current density in a PEMFC model under different temperatures, ranging from 303.15 K to 363.15 K. This analysis was conducted at a different fuel flow rate (Table 1) and the optimized fuel feed rate of 200-100 mL/min (designated as case III) and a voltage of 0.1 V results are discussed herein in detail.

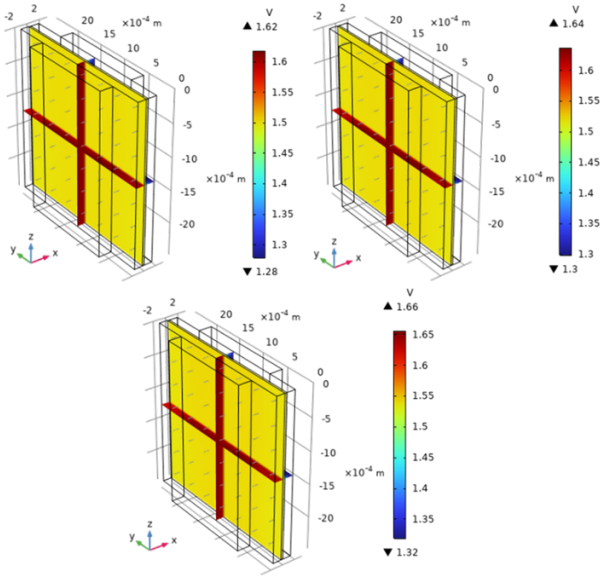

Figure 4. Distribution of electrolyte potential and electrolyte current density vector at temperature of 303.15 K, 333.15 K and 363.15 K, Flow rate: 200-100 mL/min (case III) and Voltage: 0.1 V. Multislice: Electrolyte potential (V) & Arrow volume: Electrolyte current density vector.

It is discerned from the results that the electrolyte potential exhibits a gradual increase with rising temperature. This suggests an improvement in mass transport, attributed to enhanced ion mobility. In Figure 5, we present the mass distribution of anode fuel (hydrogen) and cathode fuel (oxygen). The findings confirm a uniform distribution of both hydrogen and oxygen throughout the cell, underscoring effective fuel supply.

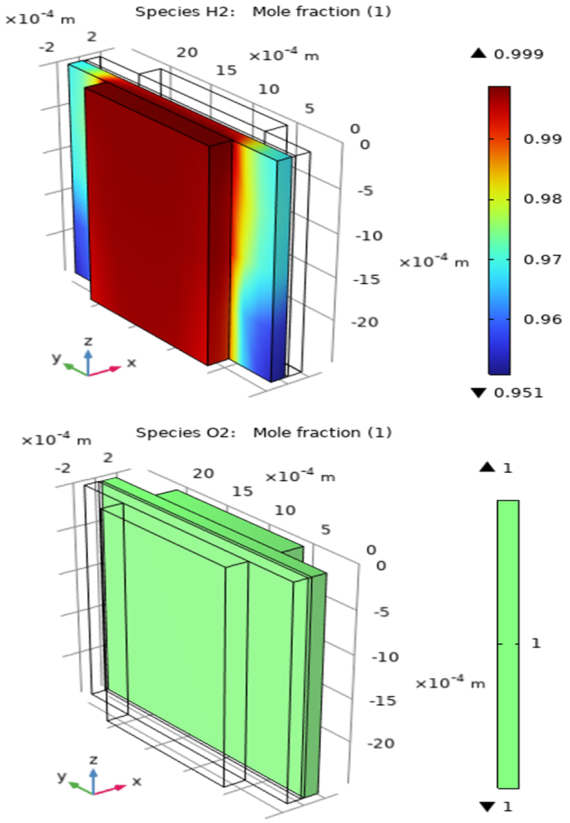

Figure 5. Mass distribution of Hydrogen and oxygen at 363.15 K at a voltage and flow rate of 0.1 V and 200-100 (H_2-O_2) mL/min

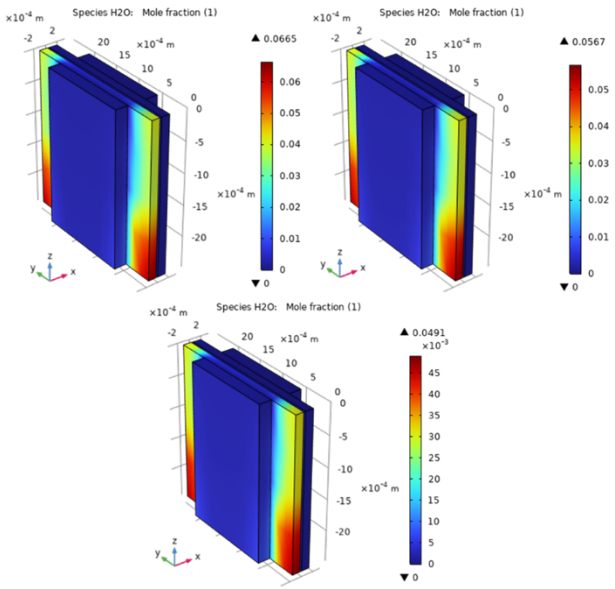

Figure 6. Mass distribution of H_2O at a voltage and flow rate of 0.1 V and 200-100 (H_2-O_2) mL/min at 303.15 K, 333.15 K and 363.15 K.

Figure 6 displays the distribution of H_2O within the PEMFC, observed over a temperature range

spanning from 303.15 K to 363.15 K, at a constant voltage of 0.1 V, and with a fuel flow rate ranging from 200 to 100 mL/min (referred to as Case III) for both hydrogen and oxygen.

From the data presented in Figure 6, it is evident that as the temperature of the PEMFC model is elevated from 303.15 K to 363.15 K, the production of water vapor as a result of electrochemical reactions gradually diminishes (measuring 0.0665 at 303.15 K, 0.0567 at 333.15 K, and 0.0497 x 10^{-3} at 363.15 K). This trend suggests that at higher temperatures, water vapor generated within the PEM fuel cell may undergo more rapid diffusion through the PEM and into the gas streams. This heightened diffusion, in turn, leads to an increased rate of water loss from the fuel cell, resulting in a decrease in water vapor formation within the cell.

Furthermore, this decline in water formation can be attributed to both the reduction in humidity within the cell and the evaporation of water vapor driven by the elevated temperature.

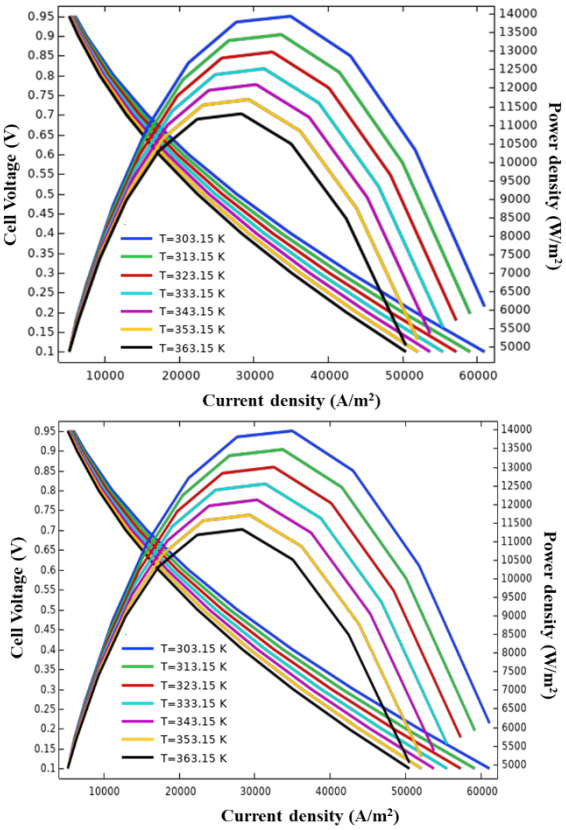

Figure 7. Polarization and Power Curves of Modeled PEMFC at different H_2-O_2 Flow Rates (100-200 & 200-100) and Temperatures (303.15 K- 36.15 K).

To investigate the impact of different fuel flow rates, an extensive parametric study was conducted, spanning a wide range of operating temperatures (303.15 K-363.15 K). Analysis of the polarization and power curves revealed a consistent trend: as the temperature increased, both current density and power density exhibited gradual decreases across all the employed fuel flow rates. The highest current density and power values were achieved under optimized conditions with an H_2:O_2 ratio of 200:100, yielding 61049 A/m^2 and 13966 W/m^2 at 303.15 K. The variations in current and power density values observed while altering the fuel flow rates can be attributed to fuel starvation, reduced water vapor for proton conduction or flooding issues, which can restrict the efficient transport of reactants within the fuel cell. The decline in current and power density with rising temperature is primarily due to the low concentration of water vapor (0.001 mol%) employed in the model. These dry conditions within the cell hinder proton conduction, subsequently limiting current density. The availability of water vapor is vital for facilitating proton transport within the cell, and at elevated temperatures, the reduced water content negatively affects this crucial aspect of the fuel cell's performance.

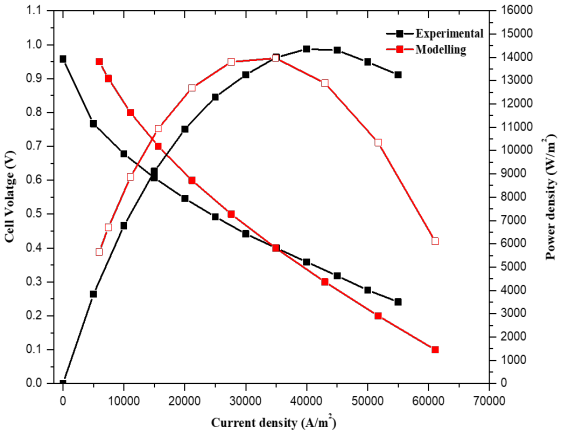

Figure 8. Comparison of Experimental and Simulation Results: Polarization and Power Curves of PEMFC at 303.15 K.

Figure 8 shows the experimental data of polarization and power curve of a PEM fuel cell, which was measured at 303.15 K while operating at a fuel flow rate of 200-100 mL/min for the H_2-O_2 mixture, under conditions where water content is limited (referred to as "dry conditions"). From figure 8, It is significant that the simulated and experimental data are matching well. This close correspondence affirms the precision and reliability of the constructed PEMFC model. In other words, the model effectively replicates the behavior of the actual fuel cell under the given operating conditions. This validation is a pivotal step in showcasing the model's effectiveness for predictive and analytical purposes in PEMFC research.

Conclusions

This comprehensive study systematically investigated the influence of diverse fuel flow rates, encompassing varying H_2:O_2 ratios (specifically, 100:100, 100:200, 200:100, and 200:200). It meticulously tracked critical performance metrics, including cell voltage, current density, power density, and overall efficiency. Furthermore, the distribution of various species, pressure profiles, and velocity profiles was analyzed, revealing a uniform

distribution of anode and cathode fuel throughout the PEMFC model. Notably, the distribution of H_2O within the PEM fuel cell exhibited a gradual decline with increasing temperature. This resulted in diminished water vapor production, which, in turn, led to a reduction in current density due to accelerated diffusion of water vapor through the PEM and into the gas streams.

Moreover, the polarization and power curves illustrated that as the PEMFC's temperature escalated, there was a consistent decline in both current density and power density across all the applied fuel flow rates. These fluctuations in current and power density were attributed to factors such as fuel starvation, reduced water vapor availability for proton conduction, and potential flooding issues, all of which could impede the efficient transport of reactants within the fuel cell.

A significant finding of this study is the strong agreement between the simulated and experimental data. This close alignment emphasizes the accuracy and reliability of the constructed PEMFC model and also confirms its effectiveness in replicating the real-world behavior of the fuel cell under the specific operating conditions examined. Such validation is a crucial milestone in establishing the model's utility for predictive and analytical purposes within the realm of PEMFC research.

References

[1] Lingchao_Xia et al., "Investigation of parameter effects on the performance of high-temperature PEM fuel cell", International Journal of Hydrogen Energy, pp. 23441-23449, 2018.

[2] Zhang, Caizhi, et al. "Determination of the optimal operating temperature range for high temperature PEM fuel cell considering its performance, CO tolerance and degradation." *Energy conversion and management*, pp. 433-441,2015.

[3] Zhou, Fan, et al. "Experimental investigation of carbon monoxide poisoning effect on a PBI/H_3PO_4 high temperature polymer electrolyte membrane fuel cell: Influence of anode humidification and carbon dioxide." *International Journal of Hydrogen Energy, pp.*14932-14941, 2015.

[4] Tiss, Faysal, Ridha Chouikh, and Amenallah Guizani. "Dynamic modeling of a PEM fuel cell with temperature effects." International journal of hydrogen energy, pp. 8532-8541, 2013.

Acknowledgements

The authors wish to thank the Department of Science and Technology [Grant no: DST/TMD/HFC/2K18/64 (G)], Government of India, New Delhi; and Indian Oil Corporation Limited [Grant no: CHT/SD-IOCL/12-01], for extending financial support towards this research work.