Analysing PEM Fuel Cell Parameters and Predicting them using Machine Learning Algorithms

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Abstract - Proton Exchange Membrane Fuel Cell (PEMFC) also known as Polymer Electrolyte Membrane Fuel Cell is one of the cleanest and most efficient energy conversion devices. PEMFC is expected to play a very big role in future energy solutions. PEM Fuel Cells work by converting the chemical energy of a fuel which is mainly hydrogen directly into electrical energy which can be used for running various electrical appliances. This is achieved by the reaction of hydrogen with oxygen over a catalyst such as Platinum and water is obtained as the by-product. PEM Fuel Cells are very promising electrochemical devices because they are highly efficient, have high power density and low emissions. Machine learning is a methodology that trains a certain model to obtain a certain data-fitting model based on the existing data fed to it and uses this model to execute predictions with high nonlinear problem forecasting accuracy and with higher computational efficiency. Machine learning models are widely used to predict parameters of various energy conversion devices. PEM Fuel Cell is also one of those devices with parameters like fuel cell performance, efficiency being accurately predicted by machine learning algorithms.

Index Terms - Energy, Fuel Cell, Hydrogen, Machine Learning, PEM

I. INTRODUCTION

The Proton Exchange Membrane used in PEM Fuel Cell is made up of a material like Perfluorosulfonic acid polymer (PFSA) that allows charged molecules which are also called ions to travel through the membrane, that separates the fuel (which is hydrogen) from the oxidant (air or oxygen). In a proton-exchange membrane fuel cell, catalysts are used in the catalyst layers (CL) to speed up and direct chemical reactions. The working principle of a PEM Fuel Cell is shown in Fig.1. At the anode, the platinum catalyst splits hydrogen molecules into protons and electrons. At the cathode, the platinum catalyst reacts with protons from the anode to reduce oxygen, producing water. The catalyst employed generally consists of Platinum (Pt) and Pt-alloy nanoparticles, while the catalyst supports are usually made of high specific surface carbons such as Vulcan carbon, ordered porous carbon, hollow graphitic particles, etc. Right now carbon-supported Platinum materials are the most recommended catalysts for PEM Fuel Cells as it has the highest catalytic activity for oxygen reduction reaction (ORR) at cathode side and hydrogen oxidation reaction at anode side. Platinum is an expensive element and due to its use as an electrolyte material has caused the cost of PEM Fuel Cells to rise and this has become one of the major challenges for their commercialization [1].

There are a number of parameters governing the performance and behaviour of PEM Fuel Cells including factors such as cell voltage, current density, temperature, humidity levels, and electrochemical impedance. Achieving optimal performance requires not only accurate measurement and monitoring of these parameters but also the ability to predict and analyse their behaviour under diverse operating conditions.

Fuel cells are categorised based on the type of electrolytes employed, with notable divisions including polymer electrolyte membrane (PEM) fuel cells (PEMFCs), solid oxide fuel cells (SOFCs), alkaline fuel cells (AFCs), phosphoric acid fuel cells (PAFCs), and molten carbonate fuel cells (MCFCs). Among these, PEMFCs are one of the best choices for vehicular applications, boasting advantages such as high electrical energy conversion efficiency, elevated power density, low operational temperatures, and rapid startup capabilities. PEMFCs are mainly composed of a Proton exchange membrane, catalyst layer (CL), gas diffusion layer (GDL), and bipolar plate (BP) [2].

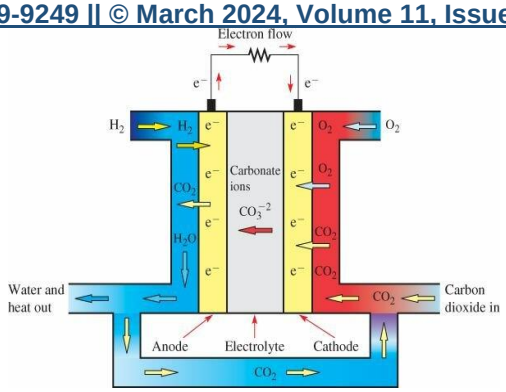


Fig. 1. Working of a PEM Fuel Cell

Traditionally, predicting and analysing PEM Fuel Cell parameters have been challenging tasks, which used to often rely on empirical correlations, complex mathematical models, and extensive experimental testing. However, these approaches are limited by their reliance on simplifying assumptions, computational inefficiency, and the sheer complexity of the underlying physical and chemical processes.

Machine learning is a method that applies model training to obtain a certain data-fitting model based on existing data and uses this model to execute predictions with high nonlinear problem forecasting accuracy and computational efficiency. Machine learning models are widely used to predict fuel cell performance, ageing, and fault diagnosis [2][3].

Enter machine learning (ML), a transformative paradigm that holds the promise of revolutionising the predictive modelling and analysis of PEM Fuel Cell parameters. ML algorithms offer a data-driven approach that can extract intricate patterns and relationships from large datasets, enabling more accurate and efficient predictions of fuel cell behaviour [3].

Machine learning (ML) is an innovative paradigm which will significantly revolutionise the predictive modelling and analysis of PEM Fuel Cell parameters. ML algorithms present a data-focused approach that enables the identification of intricate patterns and correlations in large datasets. This facilitates improved precision and efficiency in predicting the behaviour of fuel cells.

The integration of ML into PEM Fuel Cell research represents a paradigm shift, empowering researchers to overcome the limitations of traditional methods and unlock new insights into fuel cell performance. By leveraging advanced ML techniques such as regression, classification, clustering, and neural networks, researchers can develop predictive models that capture the complex interplay of factors influencing fuel cell operation.

One of the biggest advantages is that ML algorithms have the potential to adapt and learn from new data, enabling continuous improvement and refinement of predictive models over time. This adaptability is particularly valuable and comes in handy in the context of PEM Fuel Cells, where operating conditions do vary widely, and real-time adjustments are necessary to optimise performance and efficiency.

In this paper, we explore the role of machine learning in predicting and analysing PEM Fuel Cell parameters, with a focus on the challenges, methodologies, and opportunities associated with this interdisciplinary endeavour. By elucidating the benefits of ML-driven predictive modelling and analysis, we hope to inspire further research and innovation in this exciting field. Ultimately, our goal is to contribute to the development of cleaner, more efficient, and more sustainable energy solutions powered by PEM Fuel Cells.

II. PEMFC PARAMETERS

There are various physical parameters that govern the functioning of a PEMFC, those parameters are defined in detail here:

(1) Fuel Cell Temperature: The operating temperature of a fuel cell is considered to be one the most crucial factors in a fuel cell operating system. Various parameters of a fuel cell like current density, membrane conductivity, synthesis of input gas streams, and water vapour pressure are influenced by the fuel cell temperature [4].The kinetics of the PEMFC is also influenced by the operating temperature of the fuel cell, the current density increases as the fuel cell temperature rises [5] .The operating temperature of fuel cell must be in a suitable range so that a constant electrochemical reaction rate can be obtained and corrosion of PEMFC materials can be avoided. If the fuel cell is operated at high temperature, then the membrane can dehydrate or it can decompose which will result in a decreased cell voltage and hence the performance and efficiency of the PEM Fuel Cell will eventually decrease. Optimum temperature range for this fuel cell lies between 65-85 °C [6] and we have taken 70 °C for our calculations.

(3) Number of cells: Proton exchange membrane Fuel Cell (PEMFC) will play a very crucial role in upcoming years because it has high power density, quiet operation and low operating temperature. One of the applications of PEMFC is to be used as a mini portable power supply for which PEMFC is usually assembled as a stack of many cells [7]. A single PEM Fuel Cell does not generate enough voltage to be used for experiments or for practical applications so generally a number of individual fuel cells are stacked to generate enough voltage. A stack of 5 fuel cells is considered for this research.

(4) No load voltage: The no-load voltage which is also known as open circuit voltage is the voltage drawn when zero current is drawn from the supply Theoretically, no - load voltage at normal temperature and pressure or at NTP condition should be equal to 1.23 Volts. We have taken No load voltage as 1.229 Volts for this research.

(5) Hydrogen time constant: The calculation for hydrogen time constant is carried out by using the equation [8][9]

$\tau_{H2} = V_{an} / K_{H2} R$ T

Here V_{an} stands for the volume of the anode R is universal gas constant and T stands for Temperature. τ_{H2} denotes the hydrogen time constant with a value of 3.37 seconds [10].

(6) Membrane thickness: Membrane thickness is one of the most important parameters for designing a fuel cell. Various properties of fuel cells are influenced by the membrane thickness. Generally, there are two advantages of using thinner membranes, first is increased conductivity and the other one is reduced cost. These two advantages have resulted in the shrinking of membrane thickness over the time [11]. Hence it is very crucial to select an appropriate membrane thickness and hence thickness of 0.0178 cm has been selected for this research [12].

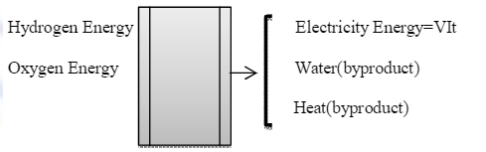
(7) Active Area: The electrochemically active part of the electrode which can produce electricity from the fuel supplied to it is referred as the Active area. The performance and the local transport processes are influenced by the active area of the fuel cell [13]. The PEM Fuel Cells could be fabricated at different active areas for specific applications. Increasing the active area of the PEM Fuel Cell increases the cell power, but not in a proportional manner [14]. The PEM Fuel Cell active area for this research is 50.6 cm^2.

(8) Reformer time constant: A reformer's function is to produce the hydrogen gas from fuels and provide it to the stack [15][16]. To control the hydrogen flow according to the output power from the fuel cell, feedback from the stack current is considered. A reformer time constant of 2 seconds is taken for this research [17][18].

(9) Electrical Resistance: The electrical resistance of a PEM Fuel Cell (proton-exchange membrane fuel cell) is the total resistance of the cell, and this resistance is determined by varying current densities and relative humidity (RH) conditions [19][20]. Also, the electrical contact resistance is a key parameter for optimising both the bipolar plate of the polymer electrolyte membrane fuel cell (PEMFC) and the electrical contact of the power terminal of the stack. The contact resistance is affected by the conductivity, roughness, and hardness of the two contacting surfaces [21][22].

(10) Max Current Density: Current density is the amount of charge that flows through a unit area in a unit of time. The limiting current density of a proton exchange membrane (PEM) fuel cell is the maximum current that can flow through an electrode [23][24]. Max current density is 1.5A/cm^2 for this research [25].

(11) Hydrogen Oxygen fuel ratio: This parameter is very crucial and affects the efficiency and working of a fuel cell. Typically, the oxygen stoichiometric ratio is 2:2.5 and the hydrogen to oxygen flow ratio in a fuel cell is typically 1.1 to 1.5 for hydrogen and 2 or more for air. The PEM Fuel Cell is operational at room temperature, but the typical operating temperature is 60 °C to 80 °C. Also, the performance of fuel cells is greatly influenced by the operating pressure. Hydrogen Oxygen fuel ratio for this research is 1.168.



(12) Fig.2. Basic Energy Conversion of a Fuel Cell

(13) Molar flow of methanol: Molar flow rate is the number of moles of a substance that passes a reference plane within a unit time interval. Methanol is a volatile, colourless, flammable, poisonous liquid with a distinctive odour. It's also known as methyl alcohol or wood alcohol. Methanol is used in many products, including fuel for internal combustion engines, boating stoves, and camping. Methanol is used for producing. Methanol contains more hydrogen than compressed or liquified hydrogen. Molar flow of methanol is 0.0002 kmol/s for this research.

(14) Fuel Cell Efficiency: Fuel cell efficiency is perhaps the most important parameter of our research as all of the input work and research carried out around the globe focuses primarily on increasing the efficiency of a fuel cell to maximise the output power gain. Fuel cell efficiency is basically the ratio of electricity produced to the amount of hydrogen consumed for the process. Fig. 2. gives the basic energy conversion of the fuel cell. Fuel cells can operate at very high efficiencies when compared with the combustion engines. Generally, fuel cells can have efficiencies up to 60% which is generally higher than 30-35% of conventional combustion-based power plants. Also Increasing the maximum current density could increase the peak power output and increase the working efficiency [26][27][28].

(15) Hydrogen Partial Pressure: Partial pressure is the pressure exerted by a gas in a mixture of gases, assuming that gas alone occupies the volume of the mixture at the same temperature. Hydrogen partial pressure is the contribution of the hydrogen gas to the total pressure [29]. Also, the output fuel cell voltage will increase as the rate of reaction increases but the partial pressure of hydrogen cannot be increased above a certain limit as it may break the membrane of the cell [30].

(16) Water partial pressure: The final product of Hydrogen PEM Fuel Cells is water which is produced by the reaction of hydrogen with oxygen and this is a highly exothermic reaction. The transportation of this product can hence greatly affect the performance of the cell. In a typical hydrogen fuel cell, each kilogram of fuel produces 9 kg of water. In a fuel cell, water vapour condensation occurs when the partial pressure of water vapour exceeds the saturation pressure. The water vapour partial pressure at the exit of a proton exchange membrane (PEM) fuel cell at 80°C is 95% of the saturated vapour pressure at 80°C [31][32].

(17) Oxygen Partial Pressure: The oxygen partial pressure in a fuel cell has a great influence on its voltage and power. A fuel cell may lose its voltage and power due to low oxygen partial pressure. Also, low oxygen partial pressure can also lead to oxygen starvation and cell reversal, which can be very harmful for the stack. A higher oxygen partial pressure can improve fuel cell performance. The oxygen partial pressure increases inside the cathode of the stack as the air mass flow increases. The oxygen partial pressure also increases with increasing the current density and decreasing the flow rate of hydrogen at the same current density [33][34][35][36].

(18) Activation losses: Activation losses in fuel cells are the voltage required to overcome the electrochemical reaction's activation energy on the catalytic surface. Three major types of fuel cell losses: – Activation losses (losses due to the electrochemical reaction) – Ohmic losses (losses due to ionic and electronic conduction) – Concentration losses (losses due to mass transport). Ohmic loss, also known as IR loss, is a voltage loss in fuel cells that is caused by resistance to the flow of electrons in electrodes, protons in electrolytes, or ions in electrolytes Concentration loss in volts is a loss of voltage that occurs when the net current density is not zero [37][38].

III. DATA COLLECTION

The data collected to perform the machine learning task has been collected using an open-source software "OPEM" [39]. The

Fig.3. OPEM software v1.3

OPEM software is a data simulation software that has been particularly developed to simulate PEMFC data and a modelling tool for evaluating the performance of proton exchange membrane fuel cells. Version 1.3 has been used. The software has a windows command prompt-based user interface as shown in Fig. 3.

It offers various static as well as dynamic models. These are mathematical formula-based models that generate data for a given set of input parameters, and output another set of PEMFC related parameters. The type of models offered in the version used as well as their names are given in Table 1.

The mathematical model used for the research carried out in this paper is the *Padulles Amphlett Analysis* model shown in Fig. 4. The model shown takes into account various input parameters like the starting and ending current, current density, temperature of O2, H2 and H2O compounds used in the fuel cell as well as various others, totalling up to 22. All the parameters are named in Table 2 along with their symbols, unit as well as the values taken.

S.No.	TYPE OF MODEL	MODEL NAME
1	Dynamic	Chakraborty Analysis
2	Dynamic	Padulles Amphlett Analysis
3	Dynamic	Padulles Analysis I
4	Dynamic	Padulles Analysis II
5	Dynamic	Padulles Hauer Analysis
6	Static	Amphlett Analysis
7	Static	Chamberline Kim Analysis
8	Static	Larminie Analysis

Table 1. Type of Model and Model Name offered in OPEM Software

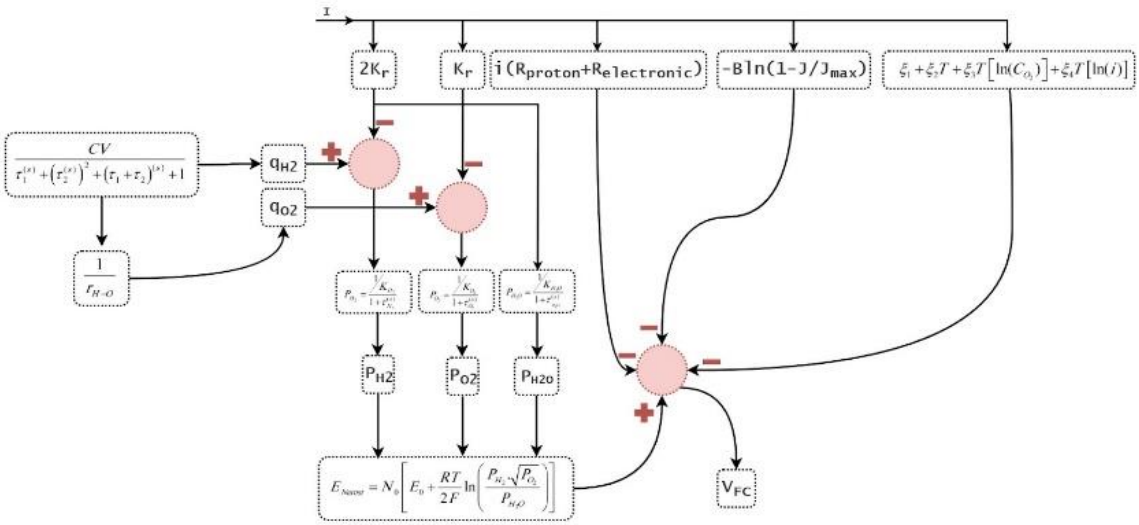


Fig. 4. Padulles Amphlett Dynamic Analysis Block Diagram

These values used can be input in two ways in the OPEM software, either entering your own values or by inputting a default vector. This default vector has been set up in such a way that the simulated values can be considered favourable and ideal.

On inputting these parameter values, a total of 13 output values are generated, including Fuel Cell Efficiency that we are trying to predict. The total number of rows in the output data file are 750.

$$istop/istep = 75/0.1 = 750$$

Hence, the dimension of the final dataset is 749×13. These output Parameters along with their units are given in Table 3.

S.No.	NAME	SYMBOL USED	VALUES TAKEN	UNIT
1	Fuel cell temperature	T	343	K
2	Number of cells	N_0	5	-
3	No load voltage	E_0	1.229	V
4	Hydrogen valve constant	K_{H2}	4.22e-05	$kmol.s^{-1}.atm^{-1}$
5	Water valve constant	K_{H2O}	7.716e-06	$kmol.s^{-1}.atm^{-1}$
6	Oxygen valve constant	K_{O2}	2.11e-05	$kmol.s^{-1}.atm^{-1}$
7	Hydrogen time constant	τ_{H2}	3.37	s
8	Water time constant	τ_{H2O}	18.418	s
9	Oxygen time constant	τ_{O2}	6.74	s
10	Membrane thickness	l	0.0178	cm
11	Active area	A	50.6	cm^2
12	Reformer time constant	τ_1	2	s
13	Reformer time constant	τ_2	2	s
14	Conversion factor	CV	2	-
15	Resistance (Electronic)	$R_{Electronic}$	0	Ω
16	An adjustable parameter with a possible minimum value of 14 and a maximum value of 23	λ	23	-
17	Maximum current density of the cell	J_{Max}	1.5	Acm^{-2}
18	Hydrogen-Oxygen flow ratio	r_{h-o}	1.168	-
19	Molar flow of methanol	$q_{methanol}$	0.0002	$kmol.s^{-1}$
20	Cell operating current start point	i_{start}	0.1	A
21	Cell operating current step	i_{step}	0.1	A

22	Cell operating current endpoint	i_{stop}	75	A

Table 2. Input Parameters in Padulles Amphlett Analysis: Symbols and Units

S.No.	Name	Unit
1	Current	A
2	Voltage	V
3	Eta Activation	V
4	Eta Concentration	V
5	Eta Ohmic	V
6	FC Efficiency	-
7	FC Power	W
8	FC Voltage	V
9	Loss	V
10	H_2 Partial Pressure	atm
11	H_2O Partial Pressure	atm
12	O_2 Partial Pressure	atm
13	Power-Thermal	W

Table 3. Output Parameters and their Units

IV. MACHINE LEARNING

Due to the amount of data collected and the type of regression analysis that should be undertaken, the machine learning algorithm: Random Forest Regressor, an ensemble model is most suitable.

Random Forest (RF) is composed of many hundreds if not thousands of decision trees. Each decision tree tries to predict a value for a subset of the given training data, then an average of each tree is taken for the final decision by the RF [40]. Breiman et al [41] first introduced the decision trees in 1984. The decision tree grows on its own during the training phase, it does not depend on any hyper parameter to decide the number of nodes, leaves or any other parameter. Thus, it is a nonparametric type of model. Each decision tree is composed of internal nodes, responsible for evaluating incoming samples through a test function, and leaf nodes. The test function assesses the features of the sample, directing it down specific branches based on the outcome. Throughout the training process, the algorithm iteratively partitions the input data at each node. This process optimises the parameters of the split functions to best align with the current data subset. Obviously, the first split, encompassing the entire dataset, is crucial as it determines the most informative variable for subsequent branching. Assuming that 'X' is the input vector having a total of 'm' features, Y is the output scalar, and 'S_n' is the training set with 'n' observations, then:

$X = \{x_1, x_2 \ldots x_m\}$, Y

$S_n = \{(X_1, Y_1), (X_2, Y_2) \ldots (X_n, Y_n)\}$, $X \in R^m$, $Y \in R$

The process of splitting input X starts at the root node, following that each node applies its own function to split the input. This is repeated recursively until a tree leaf is reached. It is common to terminate the tree when a maximum number of levels is reached. At the end of each tree, an output or predicting function ($\hat{h}$) is generated over S_n. Each tree in RF is grown according to a random subset of predictors, hence giving it its name. An L tree-structured base classifier $h(X, \Theta_k)$ is used in RF. Here, $k = 1,2 \ldots L$ and Θ_k is a set of independent, identically distributed random vectors [42].

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An ensemble method known as "Bootstrap Bagging" or just Bagging is used in RF. Bagging is a technique also proposed by Breiman in 1996 [43] which minimises variance associated with regression models, hence improving the overall prediction accuracy of a model. RF is built by randomly sampling a training data subset for each decision tree. This is known as "bootstrap", and a bootstrap sample is created by selecting n observations with replacement from S_n. The actual probability of each observation to be selected is $1/n$. The bagging algorithm picks multiple bootstrap samples ($S_n^{\Theta 1}$, $S_n^{\Theta 2}$, ..., $S_n^{\Theta q}$) and utilises the tree decision algorithm on these samples to create a set of q prediction trees, denoted as $\hat{h}(X, S_n^{\Theta 1})$,...,$\hat{h}(X, S_n^{\Theta q})$. Ensemble produces a total of q outputs in accordance with each tree. The output is given by:

$$\hat{Y} = \frac{1}{q}\sum_{l=1}^{q} \hat{Y}_l = \frac{1}{q}\sum_{l=1}^{q} \hat{h}(X, S_n^{\theta l})$$

Here $\hat{Y}_l$ is the output of l-the tree, and l = 1, 2,...,q. This framework of an RF is in Fig.5.

V. CONCLUSION

On training the RF model on the data generated from the Padulles Amphlett analysis of the PEM Fuel Cell, optimistic results have been obtained. The feature which the model has been trained to analyse is the Fuel Cell Efficiency (FCE).

The metrics used to analyse the performance of the model are:

1) The Mean Squared Error (MSE) is 1.14310-7
2) The R^2 score or the R-squared score is 0.9999834

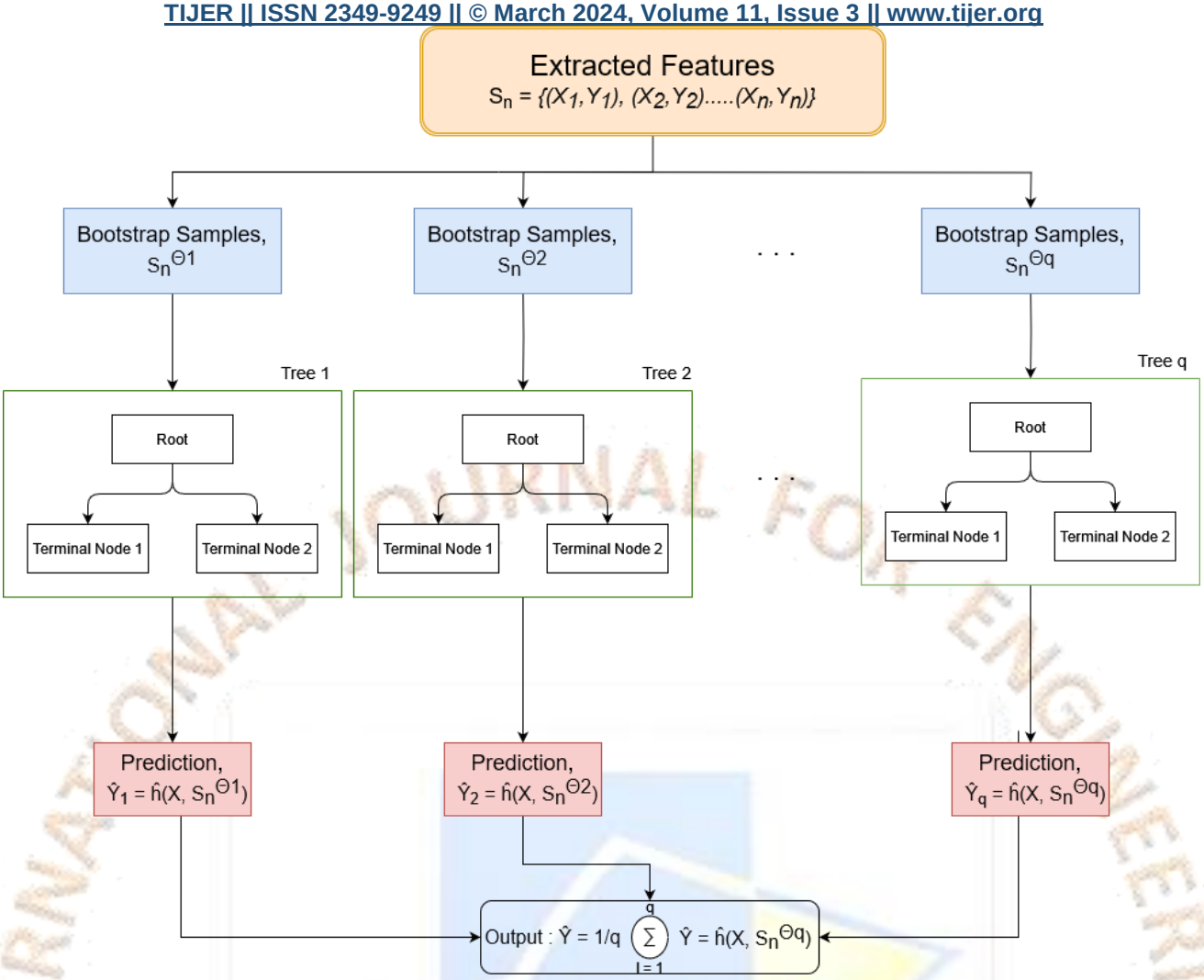

Fig. 5. Random Forest Regressor Framework

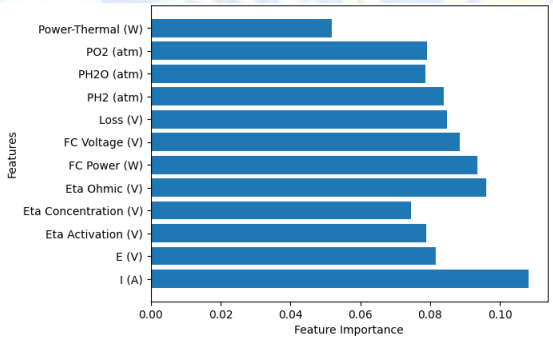

Fig. 6. Random Forest feature importance for Fuel Cell Efficiency

In the RF Regressor, feature importance is an important tool that can be utilised to understand how much each feature is contributing in the target variable, and also sheds light on what parameters will cause the most impact on the FCE. This is shown in Fig. 6.

A residual plot is a graphical tool used in regression analysis to examine the residuals or errors between the observed values and the predicted values. The residual graph calculated by the RF Regressor is shown in Fig.7.

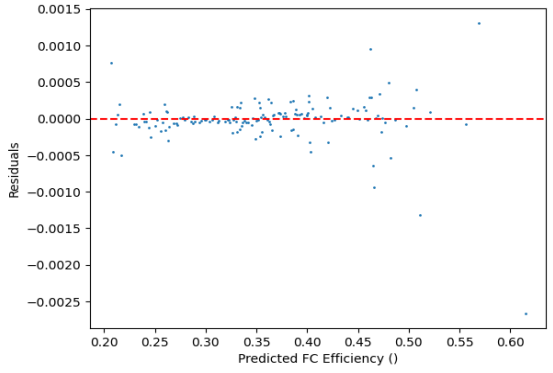

Fig. 7. Residual Plot of predicted Fuel Cell Efficiency

The research conducted in this study, gives a thorough understanding of what different parameters are instrumental in the functioning of a PEM Fuel Cell. It also underlines what parameters need improving on most to push the Fuel Cell Efficiency to the most.

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