Optimal Parameter Extraction and Performance Evaluation of Empirical Polarization Curve Model for Proton Exchange Membrane Fuel Cell

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***Abstract*—In this study, a simplified empirical polarization curve model for PEMFCs is developed. Experimental data is collected using the Nexa 1200 PEMFC test system. The model parameters are obtained through a non-linear optimization process conducted in MATLAB. The model is validated in the long run, showing a low Root Mean Square Error (RMSE), a high R^2 value, and a close match between the experimental stack voltage and the modeled stack voltage. Moreover, the variation of polarization losses (activation, ohmic, and concentration) with stack current is analyzed. In addition, the model performance is studied on reduced datasets showcasing satisfactory performance for moderate reduction, thus demonstrating the robustness and predictive performance of PEMFC under different operating conditions.**

***Index Terms*—Fuel cell, polarization curve, empirical modeling, optimization, parameter estimation.**

I. Introduction

In response to growing environmental concerns and the depletion of conventional energy sources, renewable energy technologies have become vital solutions for reducing pollution and addressing energy needs. The global transition toward renewable energy is driven by the increased cost of fossil fuel costs and concerns over greenhouse gas emissions [1].

Among the renewables, proton exchange membrane fuel cells (PEMFCs) serve as an efficient and environmentally friendly means of energy conversion. PEMFC systems are known for their high energy conversion efficiency, low noise operation, high power density, and long operational lifespan. Additionally, they offer low corrosion risk, compact design, and low operating temperatures, making them ideal for a wide range of applications. These include transportation, military operations, space missions, stationary power, and portable devices [2], [3].

The development of PEMFC models Over the past 15 years has striven to closely match the experimental setups, by employing fluid dynamics, electrochemical reactions, heat transfer, and thermal processes. Zero-dimensional models offer simplified, aggregated representations that are particularly useful for analyzing the behavior and interactions of fuel cells within power systems [3]. In PEMFC models, the electrochemical dynamics are frequently captured by semi-empirical or empirical zero-dimensional models, notably the polarization curve model (PCM). Unlike mechanistic models, these PCMs are highly favored in application-oriented studies and industrial research due to their flexibility, simplicity, and adequate accuracy [3], [4]. The polarization curve, a key performance characteristic of PEMFCs, gives the relationship between output voltage and current density. Over the years, various empirical PCMs have been developed to replicate the measured polarization curves, which are typically represented as a series of current-voltage data points. The parameters derived from these empirical models serve as crucial references for studying PEMFC performance.

Various empirical and semi-empirical PCMs of PEMFCs are developed in the literature to improve the accuracy and performance of the PEMFC model over a wide range of operations. In [5], 11 model parameters are taken into account for PEMFC modeling, however, the study does not explain in detail the calculation of partial pressures of oxygen and hydrogen. Nevertheless, a similar PCM is employed in [6]–[9], incorporating the concentration of oxygen at the cathode catalytic interface in the activation loss equation. Parameters such as contact resistance, membrane resistance, membrane thickness, electrode surface area, permanent current density, and maximum current density are not feasible to include as they vary with aging. Moreover, incorporating these may significantly increase the system complexity. These models often depend on a large number of measured parameters including reversible voltage, anode ohmic resistance, cathode ohmic resistance, limiting current density, loss current density, anode/ cathode active area, membrane thickness, Tafel slope, and exchange current density [10], [11]. This reliance on numerous parameters which are either predefined or adjusted through fitting or optimization, restricts the applicability of these models. This demands a system model relying on only limited key parameters, such as operating pressure, stack temperature, current, and voltage, to accurately capture the behavior of the fuel cell and align with empirical measure-

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ments. However, most of the research on PEMFC modeling relies on relatively small datasets for parameter optimization, generally using fewer than 60 data points. For instance, authors in [5] utilized 54 data points, in [9] 13-20 data points are considered, in [6] and [8], 60 data points and 18-29 data points are used, respectively, and authors in [7] employed 60 data points. Though the optimization problems formed are less complex, the absence of large datasets potentially limits the accuracy and robustness of the models. As a result, there is a need for larger and more comprehensive datasets to enhance the development of robust and generalized PEMFC models, to increase the model accuracy with better optimization and performance outcomes. In this study, practical data is obtained from the experimental setup of the NEXA-1200 PEMFC stack, comprising 36 cells connected in series. The key contributions are summarized as follows:

- A simplified empirical polarization curve model for PEMFC is developed, accounting for temperature and operating pressure variations throughout the polarization curve. Experiments are conducted using the NEXA-1200 PEMFC stack experimental setup to obtain practical data.
- Model parameters are estimated using a non-linear optimization method and validated on various polarization datasets.
- The proposed model incorporates parameters such as stack temperature, anode pressure, stack current, and stack voltage to accurately predict the behavior of the PEMFC, unlike models in the literature that use additional parameters such as limiting current density, maximum current density, membrane thickness, and anode/cathode surface area, etc.
- A detailed performance analysis of the model is carried out using reduced data points.

The structure of the paper is as follows: Section II outlines the simplified Empirical Polarization Curve Model. Section III details the experimental setup, the process of data collection, and parameter estimation. Section IV provides performance validation, a thorough analysis of experimental results, and performance analysis with reduced data points. Lastly, Section V offers the concluding remarks.

II. Simplified Empirical PCM

A simplified empirical model is developed in this section by making several modifications to the simpler theoretical PEMFC polarisation curve models. To distinguish model parameters from other parameters or constants, model parameters are written in boldface throughout this work. The following equation expresses the PEMFC's output voltage (V_{out}):

$$V_{out} = V_{rev} - V_{act} - V_{ohm} - V_{con} \tag{1}$$

The reversible or open-circuit voltage (V_{rev}) of a PEMFC stack depends on temperature and the partial pressures of hydrogen (P_{H_2}) and oxygen (P_{O_2}), and can be expressed as follows [12].

$$V_{rev} = N_s \left\{1.229 - 0.85 \times 10^{-3}(T_k - 298.15) + 4.3085 \times 10^{-5} T_k \ln[P_{H_2}(P_{O_2})^{0.5}]\right\} \tag{2}$$

where, T_k denotes the operating temperature of the PEMFC stack in kelvin, V_{rev} represents the open-circuit stack voltage, and N_s is the number of fuel cells present in the PEMFC stack. The Stefan-Maxwell equation for the partial pressure of oxygen and hydrogen can be represented as, [13]

$$P_{O_2} = P_{ca}\left[1 - \chi^{ca}_{H_2O} - \chi_{N_2} e^{\left(\frac{0.291J}{T_k^{0.832}}\right)}\right] \tag{3}$$

$$P_{H_2} = 0.5 P^{sat}_{H_2O}\left[\frac{e^{\left(\frac{-1.653J}{T_k^{0.832}}\right)}}{\chi^{an}_{H_2O}} - 1\right] \tag{4}$$

As the NEXA-1200 PEMFC stack operates with an open cathode, the molar fraction of nitrogen and oxygen in the cathode flow channel is assumed to be that of environmental air mixture, approximately 79% and 21%, respectively.

$$\chi_{N_2} = \frac{0.79}{0.21} P_{O_2} = 3.712 P_{O_2} \tag{5}$$

The molar fraction of water at the anode and cathode can be written as [14],

$$\chi^{ca}_{H_2O} = \frac{P^{sat}_{H_2O}}{P_{ca}} \tag{6}$$

$$\chi^{an}_{H_2O} = \frac{0.5 P^{sat}_{H_2O}}{P_{an}} \tag{7}$$

(3)-(7) involve the pressure at the anode and cathode (P_{an} and P_{ca}) in atm, the current density (J) in A/cm², the molar fraction of water ($\chi^{ca}_{H_2O}$), and the molar fraction of water ($\chi^{an}_{H_2O}$) in the anode flow channel. The exponential terms are nearly equal to one, even under conditions of low temperatures and high current densities. For instance, at the maximum current density of the PEMFC (0.413 A/cm²) and the lowest stack temperature (290 K), the exponential term is roughly 1.00104. This minimal deviation suggests that it can be safely approximated as 1 without significantly affecting accuracy. After simplification, (3) and (4) can be written as,

$$P_{O_2} = 0.212\left(P_{ca} - P^{sat}_{H_2O}\right) \tag{8}$$

$$P_{H_2} = P_{an} - 0.5 P^{sat}_{H_2O} \tag{9}$$

The relationship between the saturation pressure of water vapor ($P^{sat}_{H_2O}$) and the stack temperature (T_c) in °C can be described by [12], [15]

$$\log_{10}(P^{\text{sat}}_{H_2O}) = 2.959 \times 10^{-2}(T_c) - 9.18 \times 10^{-5}(T_c)^2 + 1.44 \times 10^{-7}(T_c)^3 - 2.1794. \tag{10}$$

Activation loss (V_{act}) in a PEMFC is associated with sluggish electrode kinetics arising from charge transfer kinetics at the electrode-electrolyte interface. The voltage decrease due to activation loss is primarily attributed to the cathode reaction [13]. The Butler-Volmer equation, used to describe activation

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loss, can be simplified to the Tafel equation as:

$$V_{act} = N_s\{(\boldsymbol{a_0} + \boldsymbol{a_1}T_k) + (\boldsymbol{b_0} + \boldsymbol{b_1}T_k)\ln I_{fc}\} \tag{11}$$

where I_{fc} is PEMFC stack current.

Ohmic losses (V_{ohm}) in PEMFCs arise due to proton and electron movement across the electrolyte and electrodes, affected by factors such as cell design, electrode materials, and operating conditions, including temperature, humidity, and current density. It can be characterized by Ohm's law as,

$$V_{ohm} = N_s I_{fc} R_{ohm} \tag{12}$$

where R_{ohm} is ohmic resistances, empirically modeled as,

$$R_{ohm} = \boldsymbol{r_0} + \boldsymbol{r_1}T_k + \boldsymbol{r_2}I_{fc} \tag{13}$$

Concentration losses (V_{con}) in PEMFCs predominantly arise from mass transport phenomena, encompassing both convection and diffusion processes. Convection involves fluid bulk movement, while diffusion pertains to species transport driven by concentration gradients, particularly governing mass transport within PEMFC electrodes [16]. At higher current densities, nitrogen buildup at the cathode can obstruct the oxygen supply, exacerbating mass transport challenges. Moreover, excess liquid water from cathodic reactions can impede reactant gas flow, further limiting mass transport efficiency [14]. Concentration loss is empirically expressed as [17], [18],

$$V_{conc} = N_s(\boldsymbol{m_0} + \boldsymbol{m_1}\,T_k)e^{\boldsymbol{n}I_{fc}} \tag{14}$$

These approaches capture the essential factors influencing polarization losses in PEMFCs, balancing complexity with practical applicability in modeling. To simplify the mathematical approach for PEM fuel cell modeling, a set of assumptions as mentioned in [13], [14], [19], [20] are considered; (i) all gases are uniformly distributed and adhere to the ideal gas law (ii) the temperatures of the fuels at the anode and cathode are assumed to be equal to the cell temperature (iii) the fuel consists of humidified hydrogen, while the oxidant comprises humidified air; for approximation purposes, the water vapor pressure at the anode and cathode are taken as 50% and 100% of saturation, respectively (iv) the parameters of individual cells are aggregated to represent the fuel-cell stack (v) the hydrogen used has a purity level exceeding 99.99%, rendering the effect of impurities negligible.

III. Experimental set-up, Data collection and Parameter estimation

The PEMFC experiment is carried out utilizing a Nexa® 1200 power module from Heliocentric, providing a power output of 1200W with voltage ranging from 16V to 40V. The stack temperature ranges from 5°C to 25°C and the maximum stack current is 60 A. An air-cooled PEMFC stack with essential peripheral components, supplied with hydrogen from a 700sl capacity metal canister is integrated, and atmospheric oxygen is supplied using cooling air. The stack comprises 36 series-connected cells with an active surface area of 149.25cm² for each electrode. The performance of PEMFCs is governed by several model parameters, given in (1)-(14). The empirical model of PEMFCs involves optimizing parameters such as $\boldsymbol{a_0}, \boldsymbol{a_1}, \boldsymbol{b_0}, \boldsymbol{b_1}, \boldsymbol{r_0}, \boldsymbol{r_1}, \boldsymbol{r_2}, \boldsymbol{m_0}, \boldsymbol{m_1}$, and $\boldsymbol{n}$ to achieve optimal performance. The model is assessed by comparing model outputs with experimental data. The objective function (OF) involves the minimization of the Sum of the Squared Error (SSE) as given below:

$$\text{SSE}(X) = \sum_{j=1}^{k} \left[V_{\text{out}}(j) - V_{\text{stack-Model}}(j)\right]^2 \tag{15}$$

$$O.F. = \text{minimize} \quad \text{SSE}(X) \tag{16}$$

where X denotes the set of ten model parameters, $V_{\text{stack-Exp}}(j)$ and $V_{\text{out}}(j)$ represents the j^{th} stack voltage from experimental and modeled data, respectively. Various quantities are recorded including system current, PEMFC current, temperatures, anode pressures, and load parameters during load variations using integrated sensors, thus providing inputs for parameter estimation. The non-linear optimization carried out using FMINCON in MATLAB utilizes each polarization dataset up to 950 data points for parameter estimation.

IV. Simulation Results Discussions

Various polarization datasets are being evaluated, and each dataset has its own set of optimized model parameters. The model parameters obtained by optimizing (16) yield SSE values ranging between 6.76V and 37.61V for each polarization dataset. Table I lists all these parameters along with their corresponding SSE values. The model parameters slightly vary in each polarization dataset due to differences in operating conditions. Table II presents the performance indices for various polarization datasets with their optimized model parameter. These indices include the Sum of Squared Errors (SSE), Normalized Root Mean Squared Error (NRMSE), Mean Absolute Error (MAE), Normalized Mean Absolute Error (NMAE), and the Coefficient of Determination (R^2). These metrics provide a comprehensive evaluation of the model accuracy in predicting the stack voltage behavior across all datasets. SSE quantifies the total deviation in predicted values of the model from the measured data, with lower values indicating better fit. NRMSE and MAE measure the error between the predicted and actual stack voltages. While MAE gives the average magnitude of errors, NRMSE normalizes the error based on the range of the data, allowing for easier comparison between datasets. NMAE is the normalized version of the MAE, providing further insight into the relative error of the model. Finally, R^2 represents the proportion of variance in the measured data explained by the model. An R^2 value closer to 1 implies the model successfully captures the underlying trends of the polarization data. The consistent performance across all datasets, particularly the high R^2 values indicates that the model is capable of accurately representing the behavior of PEMFC stack voltage under varying operational conditions.

Fig. 1 shows the comparison of reversible, measured, and modeled stack voltage with relative error for 15 different PEMFC datasets. Each subplot corresponds to a distinct

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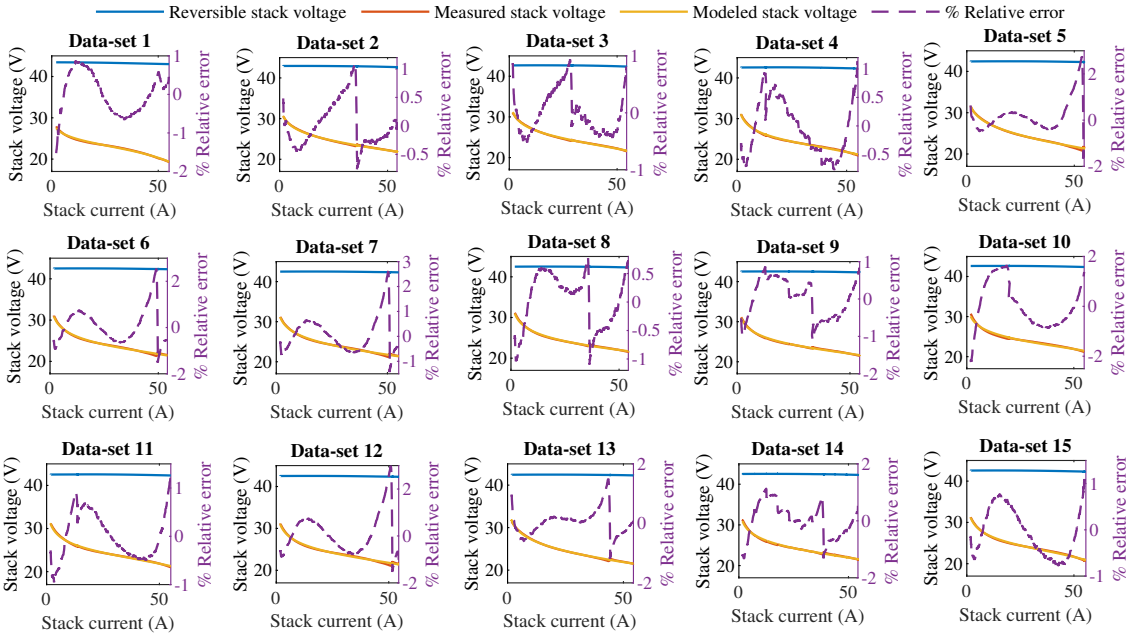


Fig. 1. Comparison of reversible, measured, and modeled stack voltage with % relative error for 15 different PEMFC datasets.

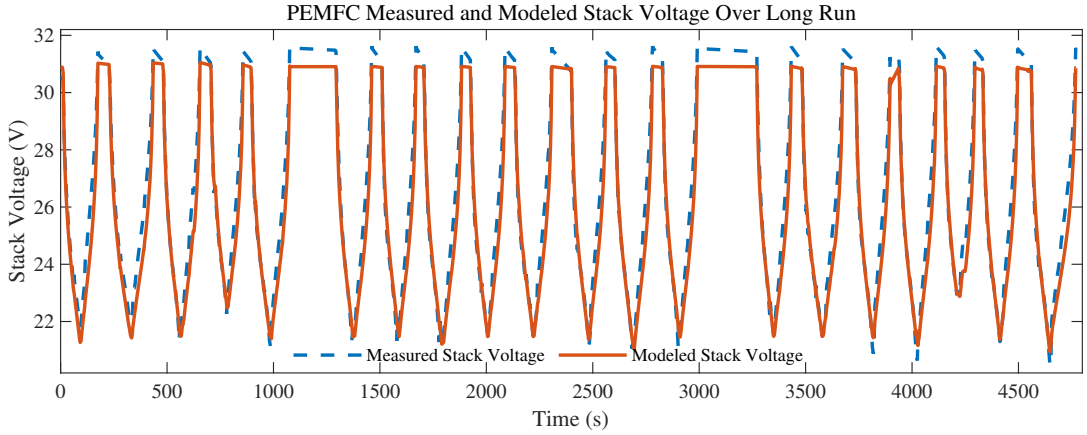


Fig. 2. Performance analysis of the PEMFC model in the long run.

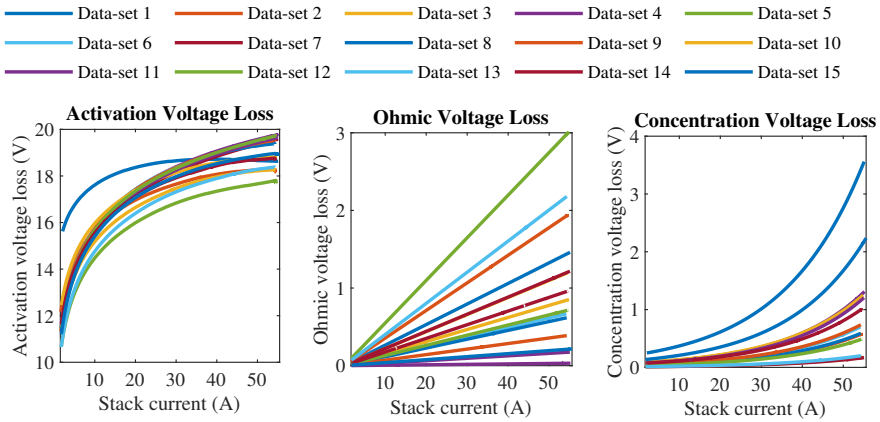


Fig. 3. Variation in polarization losses (Activation, Ohmic, and Concentration loss) with stack current.

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TABLE I

PARAMETER VARIATION DURING EVERY POLARIZATION DATASETS.

	Activation loss parameter			Ohmic loss parameter			Concentration loss parameter			Objective function value
Data-set	a_0	$a_1 \times 10^{-3}$	b_0	$b_1 \times 10^{-4}$	$r_0 \times 10^{-4}$	r_1	r_2	$m_0 \times 10^{-3}$	$m_1 \times 10^{-8}$	n	SSE
1	0.99857	-1.9976	0.096773	-2.0562	7.384	-1.3816e-08	3.9004e-08	6.3249	-2.7922e-07	0.050158	13.677
2	0.90775	-1.9245	0.083047	-0.95401	9.8776	-8.4661e-11	7.5144e-09	1.0478	-9.9521e-10	0.050026	6.7652
3	0.75144	-1.4699	0.089146	-0.95416	6.0951	-1.0062e-10	9.1032e-09	2.184	-1.1232e-09	0.050024	8.2838
4	0.29298	-0.0366	0.098	-0.95401	0.1598	-9.9478e-11	2.1664e-11	2.0671	-1.2472e-09	0.051999	13.044
5	0.93662	-2.0843	0.090645	-0.9541	15.256	-1.0675e-10	3.5453e-09	0.31399	-2.0696e-09	0.050006	21.71
6	0.77039	-1.5221	0.097988	-0.95421	3.4252	-4.541e-09	2.7286e-08	1.2957	-2.5308e-09	0.05001	20.419
7	0.27554	-2.9323	0.098	-0.954	6.1371	-2.545e-13	3.9262e-12	0.26659	-4.6126e-12	0.052	18.226
8	0.89949	-1.9278	0.098	-0.95431	3.1614	-1.559e-09	4.9198e-09	1.0843	-4.7548e-10	0.050007	11.045
9	0.66193	-1.1871	0.098	-0.95445	1.9871	-2.8511e-09	6.4675e-09	1.3299	-2.9078e-11	0.050376	13.881
10	0.99754	-2.1547	0.09649	-1.2545	4.3594	-1.5419e-08	1.2644e-08	2.8083	-1.786e-06	0.050047	37.617
11	0.27758	-2.7743	0.098	-0.954e	0.88111	-2.5801e-11	1.2364e-10	1.9121	-4.0631e-10	0.051999	10.831
12	0.28004	-2.7555	0.098	-0.954e	3.6374	-2.4472e-11	4.0795e-10	0.88681	-5.2569e-10	0.05004	26.284
13	0.87853	-1.9189	0.095673	-0.95409	11.148	-9.0223e-11	4.5007e-10	0.36644	-1.1779e-11	0.050185	9.0647
14	0.99819	-2.2127	0.096984	-1.096	4.9184	-1.1096e-08	1.3408e-08	3.3047	-4.5131e-06	0.050033	21.259
15	0.88538	-1.9166	0.09749	-0.95401	1.0787	-9.8077e-10	7.1692e-09	3.4581	-1.249e-08	0.051997	13.295

TABLE II

PERFORMANCE INDICES FOR VARIOUS POLARIZATION DATASETS WITH THEIR OPTIMIZED MODEL PARAMETERS

Data	SSE	RMSE	NRMSE	MAE	NMAE	R^2
1	13.677	0.1273	0.01468	0.10896	0.01256	0.9956
2	6.7652	0.0926	0.01069	0.07492	0.008652	0.9983
3	8.2838	0.0937	0.01000	0.07772	0.008295	0.9983
4	13.044	0.1230	0.01213	0.10927	0.01077	0.9973
5	21.71	0.1649	0.0155	0.11723	0.01105	0.9962
6	20.419	0.1675	0.01711	0.13758	0.01405	0.9946
7	18.226	0.1567	0.01564	0.12658	0.01263	0.9956
8	11.045	0.1220	0.01271	0.1049	0.01092	0.9970
9	13.881	0.1318	0.01369	0.11553	0.01199	0.9964
10	37.614	0.2271	0.0238	0.18478	0.01936	0.9872
11	10.831	0.1208	0.01191	0.10404	0.01026	0.9973
12	26.284	0.1874	0.01861	0.15433	0.01532	0.9936
13	9.0647	0.1107	0.01122	0.08193	0.008301	0.9981
14	21.259	0.1536	0.01601	0.12026	0.0125	0.9951
15	13.295	0.1301	0.01224	0.11633	0.01094	0.9973

TABLE III

PERFORMANCE RESULTS FOR DIFFERENT REDUCED DATA POINTS OF A POLARIZATION CURVE

Datapoints	RMSE	SSE	NRMSE	MAE	NMAE	R^2
50	1.2386	49413.16	0.111	1.0062	0.0902	0.7990
100	1.2435	49801.42	0.111	1.0090	0.0904	0.7974
150	1.2414	49633.49	0.111	1.0067	0.0902	0.7981
200	1.1393	41808.66	0.102	0.8856	0.0794	0.8299
250	1.2429	49758.33	0.111	1.0078	0.0903	0.7976
300	1.2432	49778.84	0.111	1.0081	0.0903	0.7975
350	1.1389	41775.36	0.102	0.9022	0.0808	0.8301
400	1.1258	40824.75	0.100	0.8723	0.0782	0.8339
450	1.2706	51998.50	0.113	1.0295	0.0923	0.7885
500	1.2458	49985.87	0.111	1.0100	0.0905	0.7967
Original	**1.1191**	**40335.88**	**0.1003**	**0.8658**	**0.0776**	**0.8359**

PEMFC dataset, showcasing the behavior of stack current versus stack voltage, under varying conditions. The reversible voltage represents the ideal stack performance, while the modeled voltage captures the prediction accuracy of the model. It is noted that the percentage relative error remains within ±2 % at all times across each polarization dataset, showing that the model gives a reliable approximation of the stack voltage performance. The average of these model parameter sets, shown in Table I, is selected to assess the long-run performance of the model. This evaluation aims to determine the model's effectiveness in predicting the fuel cell's behavior under varying operating conditions and to validate its accuracy across multiple datasets. The performance is illustrated over a continuous duration of 4800 seconds, incorporating 40 different datasets. As shown in Fig. 2, the predicted stack voltage closely aligns with the measured values, indicating the robustness of the model in long-run applications. The performance indices have the following values for the long-run: RMSE: 0.7995V SSE: 20585.2972 V, NRMSE: 0.0716, MAE:

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0.6136 V, NMAE: 0.0550, R^2: 0.9163 V. Furthermore, Fig. 3 illustrates the variation of activation, ohmic, and concentration losses with stack current for each polarization dataset.

A. Performance analysis with reduced data points

In this section, the impact of reducing the dataset size on model performance is analyzed by considering data subsets with the following number of data points: 50, 100, 150, 200, 250, 300, 350, 400, 450, and 500. The reduced dataset retains a uniform representation of the full dataset across the entire range of available data. The reduced datasets are compared with the full dataset having all the original data points. Model parameters are obtained for each data subset, and the performance metrics are calculated for each data subset, for the long run, as shown in Table III. The model parameters obtained on the full dataset exhibit the best performance, achieving the lowest error metrics with an RMSE of 1.1191V, MAE of 0.8658, and the highest R^2 value of 0.8359. It shows that the model has the highest predictive accuracy using all available data points. As the number of data points decreases, a gradual decline in performance is observed. For example, a dataset with 400 points maintains a close level of performance to the full dataset with an RMSE of 1.1258V and an R^2 value of 0.8339V. This suggests that even with a reduced data size, the generalized model can perform well without significantly losing model accuracy. However, when the number of data points is reduced to 50, 100, and 150, there is a degradation in model performance. RMSE values for these datasets range between 1.2386 and 1.2435, while R^2 values drop below 0.8. The deterioration of the error metrics suggests that reducing the dataset too much impairs the model's ability to capture the underlying patterns in the data, thus compromising the predictive performance of the model.

V. Conclusion

A simplified empirical polarization curve model for PEMFC is developed in this paper. Data collection is experimentally carried out using the Nexa 1200 PEMFC test system, and the modeling parameters are obtained using an optimization considering various polarization datasets. The non-linear FMINCON optimization process carried out in MATLAB utilizes each polarization dataset comprising up to 950 data points for parameter estimation. The model is validated for a long run of 4800s which provides low NRMSE and NMAE values and R^2 close to 1, showcasing efficient performance. The low RMSE and the close match between the experimental stack voltage and the modeled stack voltage indicate good agreement with the modeling. The variation of polarization losses with stack current is also studied. These results highlight the robustness of the model and its potential for accurately forecasting PEMFC performance across various operating conditions. Furthermore, performance analysis with reduced data points is carried out, demonstrating satisfactory performance with moderate reductions in data points. Larger reductions lead to noticeable losses in accuracy, deteriorating the predictive performance of the model.

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