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Prediction of polarization curves of PEMFC membrane electrode assembly using artificial intelligence technics

Yapay zeka teknikleriyle PEMFC membran elektrot yapısının polarizasyon eğrilerinin tahmini

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Abstract

Proton exchange membrane fuel cells (PEMFCs) are used commercially in automobiles, buses, uninterruptible power supplies, and combined heat power systems, holding a significant place in the fuel cell market. Fuel cell performance is characterized by polarization curves in design and manufacturing processes. This study predicts a PEMFC's polarization curves using comparative artificial intelligence (AI) models trained and tested under different operational conditions. The AI model inputs are cell temperature, humidity, anode-cathode flow, and membrane resistance. The outputs are cell voltage and current density. The model outputs are compared with experimental values for 50°C, 100% humidity using MATLAB software. The average Root Mean Square Error (RMSE) for the ANFIS prediction is 0.056112, while for the ANN prediction it is 0.011919. These results indicate that the Artificial Neural Network (ANN) method outperforms the Adaptive Neuro Fuzzy Inference System (ANFIS) in predicting the behavior of the PEMFC's Membrane Electrode Assembly (MEA). The models showed promising results with high accuracy.

Keywords: Artificial intelligence, Electrochemical devices, Energy conversion, Fuel cells

Öz

Proton değişim membranlı yakıt hücreleri (PEMFC) otomobiller, otobüsler, kesintisiz güç kaynakları ve kombine ısı güç sistemlerinde ticari olarak kullanılmaktadır ve yakıt hücresi pazarında önemli bir yere sahiptir. Yakıt hücresi performansı, tasarım ve üretim süreçlerinde polarizasyon eğrileri ile karakterize edilir. Bu çalışma, farklı çalışma koşullarında eğitilip test edilen karşılaştırmalı yapay zeka (AI) modelleri kullanarak bir PEMFC'nin polarizasyon eğrilerini tahmin etmektedir. AI model girdileri hücre sıcaklığı, nem, anot-katot akışı ve membran direncidir. Çıktılar ise hücre voltajı ve akım yoğunluğudur. Model çıktıları, MATLAB yazılımı kullanılarak 50°C, %100 nem koşullarındaki deneysel değerlerle karşılaştırılmıştır. ANFIS tahmini için hataların ortalama karekökü (RMSE) 0.056112 iken, ANN tahmini için 0.011919'dur. Bu sonuçlar, Yapay Sinir Ağı (ANN) yönteminin, PEMFC'nin Membran Elektrot Yapısının (MEA) davranışını tahmin etmede Uyarlamalı Nöro Bulanık Çıkarım Sistemi (ANFIS) yönteminden daha iyi performans gösterdiğini göstermektedir. Modeller yüksek doğrulukla umut verici sonuçlar vermiştir.

Anahtar kelimeler: Yapay zeka, Elektrokimyasal cihazlar, Enerji Dönüşümü, Yakıt hücreleri

1 Introduction

PEMFCs, compared with other types of fuel cells, have the highest energy density and the fastest start-up time [1]. The PEMFC is electrochemically complex and has a nonlinear nature [2]. This complex structure complicates the commercialization of hydrogen fuel cells. According to the U.S. Department of Energy (DOE)'s report, market drivers for PEMFCs include the need for methods to reduce the time and costs of final fuel cell stack tests in manufacturing [3]. Current final testing processes take a long time due to expensive equipment, limited floor space, and gas preparation [4-5]. Fuel cell modeling can lead to improvements in fuel cell design, making them more cost-effective and efficient. The model must be robust, accurate, and provide solutions for fuel cell issues.

Comparative studies of ANN and ANFIS are used to address the nonlinear statistical and complex structures of PEMFCs [6-9]. Inputs for the PEMFC model include anode and cathode flow, cell resistance, temperature, and humidity, with the output being the polarization curve. Neuro-Adaptive and Neural-Network Learning systems have been studied extensively [6-9]. This paper is organized into the following sections: Section II explains PEMFC dynamics. Section III describes the experimental setup and polarization curves of the MEAs under different conditions. Section IV explains the ANFIS architecture and performance. Section V details the ANN architecture and presents both experimental and predicted polarization curves. The final section presents conclusions.

2 PEMFC dynamics

Fuel cells are electrochemical devices that are environmentally friendly and have high energy density. Therefore, they are used as alternative power systems. Due to the complex and dynamic structures of fuel cells,

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designing and developing them is a challenging process. Figure 1 illustrates the complexity of the PEMFC system.

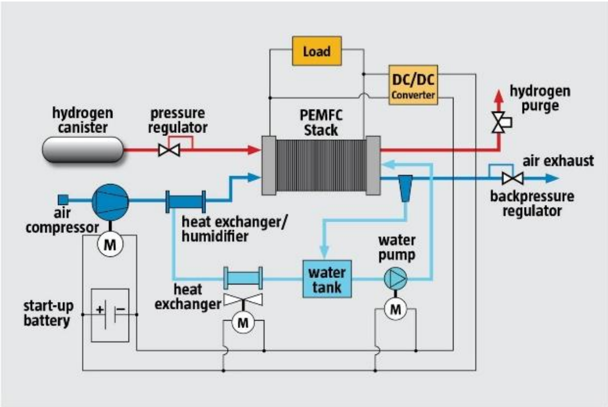

Figure 1. Working diagram of PEMFC system [10]

The key component of a PEMFC is the membrane electrode assembly (MEA), which comprises a Nafion® membrane sandwiched between electrodes, gas diffusion layers, and catalyst layers. Electrodes are typically made of woven carbon paper or cloth. The PEMFC catalyst layer is in direct contact with both sides of the membrane and consists of Pt nanoparticles supported on micron-sized carbon particles. Each gas diffusion layer (GDL) surrounds the catalyst layers and is made of carbon fibers coated with Polytetrafluoroethylene (PTFE) to impart hydrophobic properties, thereby reducing the formation of water droplets that could hinder gas diffusion to the catalyst [11-15]. All the chemical reactions in the PEMFC occur within the MEA [16]. Figure 2 illustrates the MEA structure.

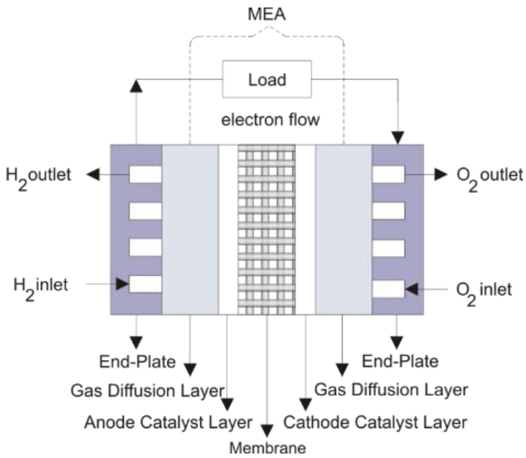

Figure 2. Membrane electrode assembly (MEA)

The complexity of the electrochemical reactions within the PEMFC's MEA contributes to the challenges of its commercialization and testing. While the single cell voltage is 1.229V, various performance losses, including activation, ohmic, and mass transport losses, lead to a decrease in overall cell voltage.

The performance of PEMFCs can be assessed and characterized using polarization curves [17-20]. These curves are essential for understanding the efficiency and operational characteristics of Proton Exchange Membrane Fuel Cells (PEMFCs). A polarization curve plots the cell voltage against the current density, revealing the various types of losses or overpotentials encountered during operation (Figure 3). These losses include activation losses, ohmic losses, and concentration losses. Activation losses stem from the kinetics of electrochemical reactions, notably the sluggish oxygen reduction reaction at the cathode. Ohmic losses result from resistance to ion flow in the electrolyte and electron flow within the cell components. Concentration losses, or mass transport losses, occur when reactants are not supplied adequately to the reaction sites, leading to a voltage drop at higher current densities. Each type of loss dominates different regions of the polarization curve: activation losses prevail at low current densities, ohmic losses in the mid-range, and concentration losses become significant at high current densities [21]. Analyzing these curves enables researchers to diagnose performance issues and refine design and material choices for PEMFCs, thereby improving their efficiency and operational longevity [22].

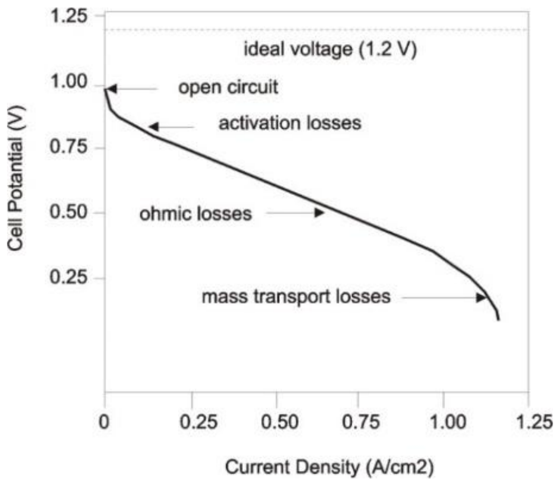

Figure 3. Polarization curve of the PEMFC

3 Experimentation of PEMFC's MEA

PEMFC's MEA is tested via Teledyne Medusa® Fuel Cell Testing System (Figure 4). PEMFC's polarization curves represent the steady-state performance achieved after 5 minutes of operation (Figure 5). Nafion® 212 is used as an electrolyte.

Figure 4. The PEMFC's MEA testing system

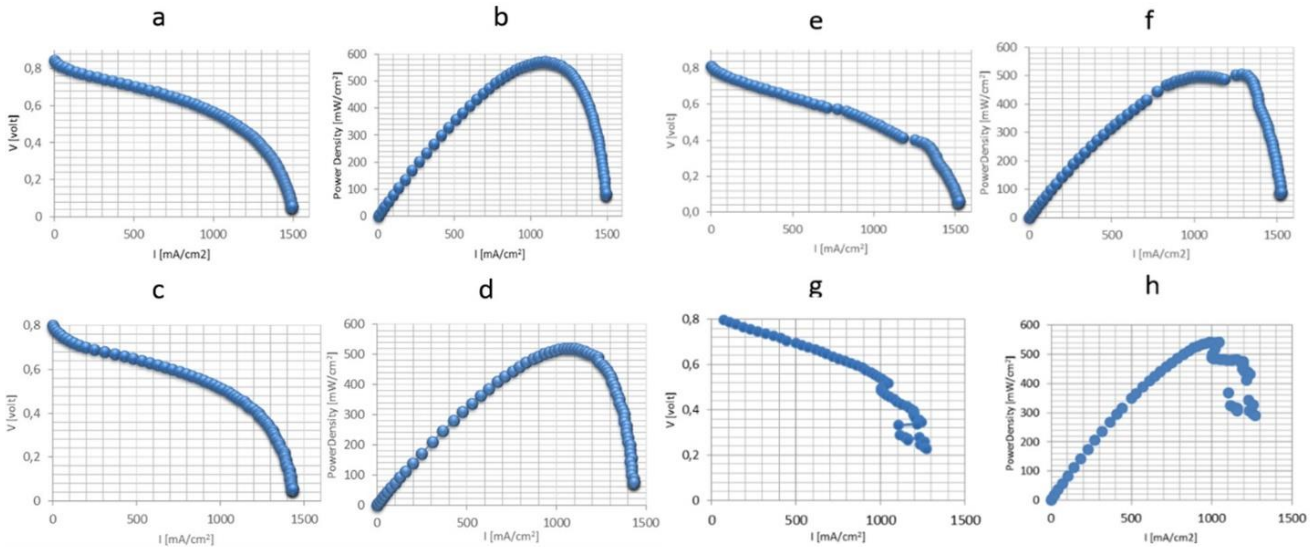

Figure 5. The polarization curves of PEMFC's MEA at different conditions. (a) Cell voltage vs. current at 50 °C temperature and 100% humidity. (b) Power density vs. current at 50 °C temperature and 100% humidity. (c) Cell voltage vs. current at 50 °C temperature and 75% humidity. (d) Power density vs. current at 50 °C temperature and 75% humidity. (e) Cell voltage vs. current at 80 °C temperature and 75% humidity. (f) Power density vs. current at 80 °C temperature and 75% humidity. (g) Cell voltage vs. current at 80 °C temperature and 100% humidity. (h) Power density vs. current at 80 °C temperature and 100% humidity

The reactions in a fuel cell occur at the anode and cathode catalyst plates on either side of the membrane. The overall reaction is similar to a combustion process, which is exothermic, releasing energy and water. This heat (enthalpy) generated from the reaction represents the difference in formation temperatures between the products and reactants. At room temperature (25°C), the reaction that produces liquid water releases an energy of ΔH = -286 kJ.mol^{-1}, known as the Higher Heating Value (HHV). However, not all of this enthalpy energy is converted into electrical energy; some is lost due to various factors. The portion of energy that is converted into electrical energy is represented by Gibbs free energy (ΔG) (Table 1).

$$\Delta G = \Delta H - T\Delta S \tag{1}$$

where H is enthalpy, T is absolute temperature, and S is entropy.

Table 1. Enthalpies, entropies and Gibbs free energy of H2/O2 fuel cell reaction in (kJ/mol.K) and the resulting theoretical cell potential at 25°C([23])

	ΔH (kJ/mol)	ΔG (kJ/mol)	ΔS (kJ/mol.K)	E (Volt)
H2 + 1/2O2 → H2O (liquid)	−285.8	−237.1	−0.163	1.23
H2 + 1/2O2 → H2O (gas)	−241.8	−228.6	−0.045	1.18

4 Architecture of proposed ANFIS model

ANFIS is formed by integrating adaptive neural networks and fuzzy logic rules, providing an effective model for nonlinear system modeling. The fuzzification layer matches the inputs according to fuzzy rules based on membership functions. Figure 6 shows the Fuzzy Inference System (FIS). All rules are evaluated on parallel surfaces in the fuzzy logic framework (fuzzification). The results of these rules are then combined and filtered (defuzzification). Adaptive networks often use supervised learning algorithms during the learning stage. These networks have several adaptive nodes directly connected to each other [21-22].

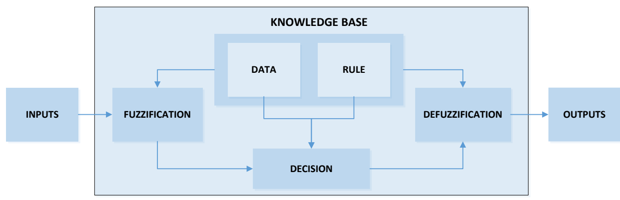

Figure 6. Fuzzy inference system (FIS)

The ANFIS consists of five layers: fuzzification, rule, normalization, defuzzification, and summation neuron layers [24]. ANFIS integrates fuzzy learning and artificial neural networks, employing different types of models. The two most commonly used types are Mamdani and Takagi-Sugeno. The basic formulation for a two-input (x, y) and one-output (f) model is as follows [24-26]. The structure of the Takagi-Sugeno-Kang ANFIS type is depicted in Figure 7.

Rule: if x is A1 and y is B1, then

$$f\_1 = p\_1\, x + q\_1\, y + r\_1 \tag{2}$$

Rule: if x is A2 and y is B2, then

$$f\_2 = p\_2\, x + q\_2\, y + r\_2 \tag{3}$$

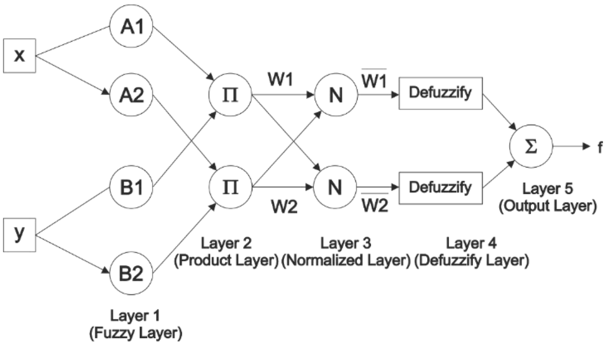

Figure 7. Structure of Takagi Sugeno-Kang ANFIS type

The Takagi Sugeno-Kang ANFIS type consisting inputs *x* and *y*, two rules and one output. Every node *i* in the layer 1 is a square node with a node function.

$$O_i^1 = \mu A_i(x) \tag{4}$$

where *x* is the input to node *i*, and A_i is the linguistic label. O_i^1 is the membership function of A*i*.

$$\mu A_i(x) = \frac{1}{1 + \left[\left(\frac{x - c_i}{a_i}\right)^2\right] b_i} \tag{5}$$

a_i,b_i,c_i are the parameter set [27-28].

In ANFIS, the Gaussian membership function was used for the input variables. There are 243 rules in the system. The learning rate used during the training process of the model is 0.05. The number of epochs is 50, and the error tolerance is 10^{-5}. The model has 5 layers.

Input Layer (Layer 1): This is the layer where the input variables (anode flow, cathode flow, resistance of the cell, cell temperature, humidity) are placed.

Membership Function Layer (Layer 2): This is the layer where the input variables are fuzzified and their membership degrees are calculated.

Rule Layer (Layer 3): This is the layer where the firing strengths of the rules are calculated based on the membership degrees.

Normalization Layer (Layer 4): This is the layer where the values from the rule layer are normalized and combined.

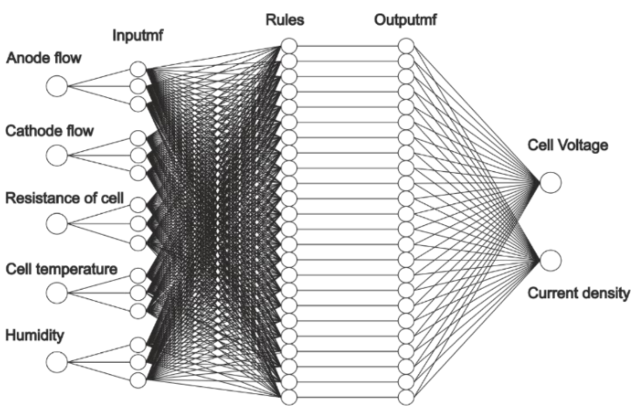

Figure 8. The ANFIS model structure

Output Layer (Layer 5): This is the layer where the outputs of the rules are calculated and the final outputs of the system (cell voltage and current density) are produced.(Figure 8). The use of two sigmoid functions in output layer yielded the best results and was implemented in this study.

Back propagation learning and least mean square estimation are utilized in the ANFIS model to determine the parameters, with the procedure iterated for optimization. The data set obtained at 100% humidity and 80 ºC is used to predict the voltage of PEMFC's MEA (Figure 9). Experimental data for PEMFC's MEA at 75% humidity and 50 ºC serves as the ANFIS training data set (Figure 10). An average root mean square error (RMSE) of 0.056112 is achieved by the 40th epoch.

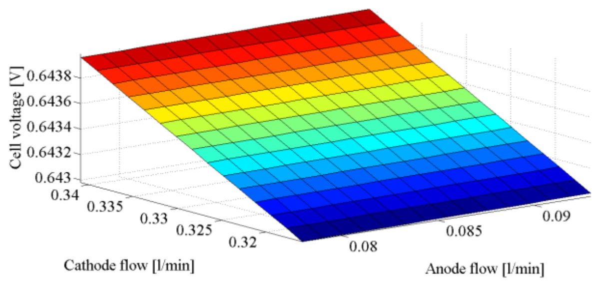

Figure 9. The cell voltage curve depends on anode-cathode flow

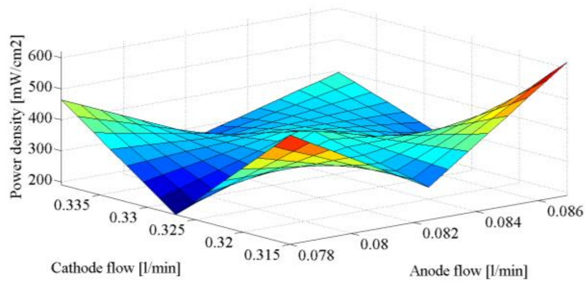

Figure 10. The power density curve of depends on anode-cathode flow

5 Architecture of proposed ANN model

ANN is a model that mimics the layered and parallel structure of the brain, which is composed of nerve cells. Like the brain, ANN can generate new information through learning. The ANN model is a powerful and reliable tool for modeling nonlinear systems. It consists of three primary network types: single-layer feedforward networks, multi-layer perceptron (MLP) feedforward networks, and recurrent networks [29]. The ANN structure used in this study includes 5 inputs, 20 hidden neurons, and 2 outputs Dataset split into 75% training, 15% validation, and 15% test. The Sigmoid activation function was used in the hidden layers and the output layer. The Learning Rate was set to 0.0005, Batch Size to 64, and the number of Epochs to 50. The number of epochs is determined based on the complexity of the model, the size of the dataset, and the learning speed of the model. The ANN network is depicted in Figure 11.

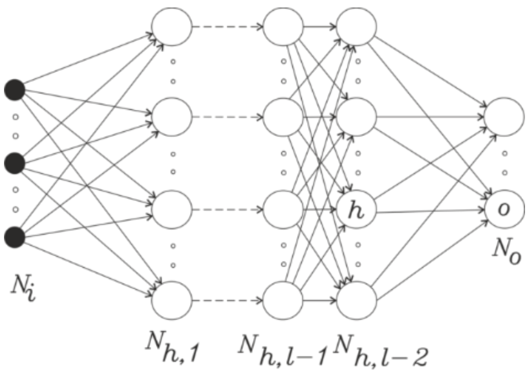

Figure 11. The multi-layer ANN network with *l* layers of units

The functioning of an ANN involves several key steps: forward propagation, loss calculation, backpropagation, and iterative training. Initially, input data is fed into the input layer, where each neuron's output is computed as a weighted sum of its inputs and then passed through an activation function. This process continues through each layer until the data reaches the output layer, producing the final prediction. The network then compares this prediction to the actual target values using a loss function, which quantifies the error. During backpropagation, the network adjusts the weights of the connections between neurons by computing the gradient of the loss function with respect to each weight and updating the weights to minimize the error. This iterative process, carried out over multiple training epochs, gradually reduces the error, enhancing the network's ability to learn underlying patterns in the data [30].

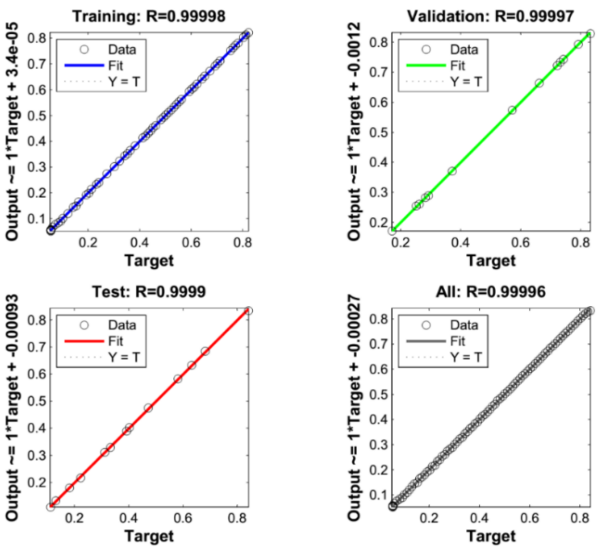

Figure 12. ANN Regression analysis

In this study, the relationship between ANN training, validation and test data and output values was examined by regression analysis. The perfect fit for regression plots should fall along a 45-degree line. In this study, the regression analysis showed is remarkable results for all data sets. R-value for each case is 0.9999 (Figure 12).

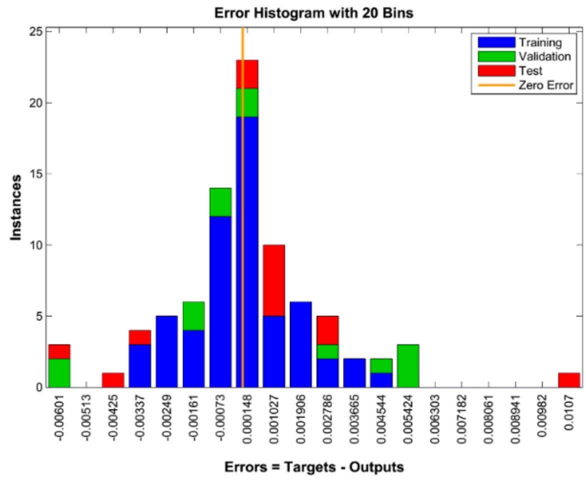

Figure 13. Error histogram for ANN model

The obtained error histogram validates the performance of the ANN network. The blue bars represent the training data set, the green bars represent the validation data set, and the red bars represent the testing data set. Most errors fall between -0.00513 and 0.006303 in the error histogram (Figure 13).

6 Conclusions

By using AI techniques such as ANFIS and ANN, the cost and time involved in the design of PEMFCs can be reduced. Unlike physical models, fuel-cell performance curves are generated with fewer variables. This study proposes ANFIS and ANN models for predicting the polarization curve of PEMFC’s MEA. The prediction performance of the ANFIS and ANN models is evaluated using RMSE.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i-1}^{n}(a_i - p_i)^2} \tag{6}$$

a_i, actual values
p_i, predicted values
The average RMSE for the ANFIS prediction is 0.056112 and the ANN prediction is 0.011919.

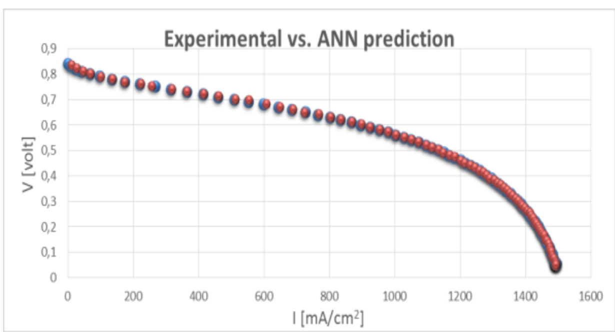

Figure 14. ANN prediction vs. experimental results

In Figure 14 and Figure 15, the red dots represent the predicted values, while the blue dots represent the experimental values.

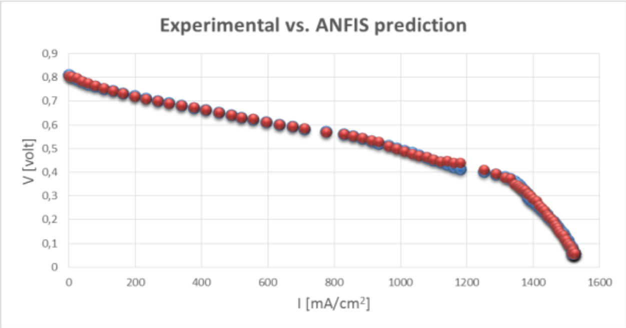

Figure 15. ANFIS prediction vs. experimental results

The existing literature frequently highlights the advantages of ANFIS in environments where interpretability and the ability to manage non-linear and uncertain data are crucial. ANFIS's integration of fuzzy logic with neural networks enables it to effectively capture complex relationships within data, providing a level of transparency through interpretable fuzzy rules. However, despite these strengths, this study demonstrates that ANN, which is relatively simpler to implement and scale, can yield more effective results in predicting complex systems like fuel cell polarization curves.

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Conflict of interest

The authors declare that there is no conflict of interest.

Similarity rate (iThenticate): %16

References

[1] V. Lakshminarayanan and P. Karthikeyan, Performance enhancement of interdigitated flow channel of PEMFC by scaling up study. Energy Sources Part A: Recovery, Utilization, and Environmental Effects, 42 (14), 1785–1796, 2019. https://doi.org/10.1080/15567036.2019.1604889.

[2] M. Wei, S. J. Smith and M. D. Sohn, Experience curve development and cost reduction disaggregation for fuel cell markets in Japan and the US. Applied Energy, 191, 346-357, 2017. https://doi.org/10.1016/j.apenergy.2017.01.056.

[3] U.S. Department of Energy, 2019 Annual Progress Report, DOE Hydrogen and Fuel Cells Program. https://www.hydrogen.energy.gov/library/annual-progress/annual_progress19, Accessed 10 January 2024.

[4] X. Lü, Y. Qu, Y. Wang, C. Qin and G. Liu, A comprehensive review on hybrid power system for PEMFC-HEV: Issues and strategies. Energy Conversion and Management, 171, 1273-1291, 2018. https://doi.org/10.1016/j.enconman.2018.06.065.

[5] L. James and D. Andrew, Fuel Cell Systems Explained. Wiley, New York, 2003.

[6] C. Spiegel, PEM Fuel Cell Modeling and Simulation Using MATLAB. Academic Press, 2008.

[7] Z. Li, S. Jemei, R. Gouriveau, D. Hissel and N. Zerhouni, Remaining useful life estimation for PEMFC in dynamic operating conditions. Proceedings of IEEE Vehicle Power and Propulsion Conference (VPPC), pp. 1-6, Hangzhou, China, 2016.

[8] Y. Vural, D. B. Ingham, and M. Pourkashanian, Performance prediction of a proton exchange membrane fuel cell using the ANFIS model. International Journal of Hydrogen Energy, 34 (22), 9181-9187, 2009. https://doi.org/10.1016/j.ijhydene.2009.08.096.

[9] M. Seyhan, Y. E. Akansu, M. Murat, Y. Korkmaz, and S. O. Akansu, Performance prediction of PEM fuel cell with wavy serpentine flow channel by using artificial neural network. International Journal of Hydrogen Energy, 42 (40), 25619-25629, 2017. https://doi.org/10.1016/j.ijhydene.2017.04.001.

[10] M. Mehrpooya, B. Ghorbani, B. Jafari, M. Aghbashlo and M. Pouriman, Modeling of a single cell micro proton exchange membrane fuel cell by a new hybrid neural network method. Thermal Science and Engineering Progress, 7, 8-19, 2018. https://doi.org/10.1016/j.tsep.2018.04.012.

[11] X. Wu, X. Zhu, G. Cao and H. Tu, Nonlinear modeling of a SOFC stack based on ANFIS identification. Simulation Modelling Practice and Theory, 16 (4), 399-409, 2008. https://doi.org/10.1016/j.simpat.2008.01.004.

[12] F. Barbir, PEM Fuel Cells: Theory and Practice. Academic Press, 2005.

[13] Q. Li, W. Chen, Y. Wang, J. Jia and M. Han, Nonlinear robust control of proton exchange membrane fuel cell by state feedback exact linearization. Journal of Power Sources, 194 (1), 338-348, 2009. https://doi.org/10.1016/j.jpowsour.2009.04.077.

[14] D. Zhou, F. Gao, E. Breaz, A. Ravey, A. Miraoui and K. Zhang, Dynamic phenomena coupling analysis and modeling of proton exchange membrane fuel cells. IEEE Transactions on Energy Conversion, 31 (4), 1399-1412, 2016. https://doi.org/10.1109/TEC.2016.2587162.

[15] D. Yu and S. Yuvarajan, A novel circuit model for PEM fuel cells. Proceedings of Nineteenth Annual IEEE Applied Power Electronics Conference and Exposition, pp. 362-366, Anaheim, CA, USA, 2004.

[16] J. Jia, Y. Wang, M. Han and Y.T. Cham, Dynamic characteristic study of proton exchange membrane fuel cell. Proceedings of IEEE Sustainable Energy Technologies, pp. 24-27 Singapore, 2008.

[17] G. S. Avcioglu, B. Ficicilar and I. Eroglu, Effect of PTFE nanoparticles in catalyst layer with high Pt loading on PEM fuel cell performance. International Journal of Hydrogen Energy, 41(23), 10010-10020, 2016. https://doi.org/10.1016/j.ijhydene.2016.03.048.

[18] N. M. Zahari and A. A. Aziz, Effect of platinum catalyst loading on membrane electrode assembly (MEA) in proton exchange membrane fuel cell (PEMFC). 10th IEEE Int. Conf. Semiconductor Electronics (ICSE), pp. 669-673, Kuala Lumpur, Malaysia, 19-21 September 2012.

[19] Y. Wang, K. S. Chen, J. Mishler, S. C. Cho and X. C. Adroher, A review of polymer electrolyte membrane fuel cells: Technology, applications, and needs on fundamental research. Applied Energy, Volume 88(4), 981-1007, 2011. https://doi.org/10.1016/j.apenergy.2010.09.030.

[20] C. Wang, M. H. Nehrir and S. R. Shaw, Dynamic models and model validation for PEM fuel cells using electrical circuits. IEEE Transactions on Energy Conversion, 20(2), 442-451, 2005, https://doi.org/10.1109/TEC.2004.842357.

[21] D. Zhou, Y. Wu, F. Gao, E. Breaz, A. Ravey and A. Miraoui, Degradation prediction of PEM fuel cell stack based on multi-physical aging model with particle filter approach. IEEE Industry Applications Society Annual Meeting, pp, 1-8, Portland, USA, 02-06 October 2016.

[22] E. Dursun, G. Y. Ozalp and O. Kilic, Experimental Analysis and Electrical Modeling of PEM Fuel Cell's MEA. International Review Of Electrical Engineering-Iree Part:A, 5, 1595-1599, 2010.

[23] L. Khotseng, Fuel Cell Thermodynamics. in: P. Vizureanu, (Eds.), Thermodynamics and Energy Engineering, IntechOpen, pp, 1-17, 2019.

[24] A. H. Abdulwahid and S. Wang, A new protection approach for microgrid based upon combined ANFIS with Symmetrical Components. 2016 IEEE PES Asia-Pacific Power and Energy Engineering Conference (APPEEC), pp, 1984-1989, Xi'an, China, 2016.

[25] S. Wayan and M.A. Kemal, Modeling of Tropospheric Delays Using ANFIS. Springer, Switzerland, 2016.

[26] B. B. Jovanovic, I. S. Reljin and B. D. Reljin, Modified ANFIS architecture - improving efficiency of ANFIS technique. 7th Seminar on Neural Network Applications in Electrical Engineering, pp, 215-220 Belgrade, Serbia, 2004.

[27] M Sugeno and G.T Kang, Structure identification of fuzzy model. Fuzzy Sets and Systems, 28(1), 15-33, 1988, https://doi.org/10.1016/0165-0114(88)90113-3.

[28] M. Alakhras, M. Oussalah and M. Hussein, ANFIS: General description for modeling dynamic objects. IEEE/ACS 12th International Conference of Computer Systems and Applications (AICCSA), pp, 1-8, Marrakech, Morocco, 2015.

[29] J.S.R. Jang, Input selection for ANFIS Learning. IEEE Int. Conf. Fuzzy Systems, pp. 1493-1499, New Orleans, LA, USA, 1996.

[30] S. Sumathi and S. Paneerselvam, Computational intelligence paradigms: theory and applications using MATLAB. CRC Press, Florida, 2010.