**A Data-Driven Framework for Prediction of Carbon Based Hybrid Catalyst Layer Performance in Polymer Electrolyte Fuel Cells using Artificial Neural Networks**

Nahid Gholami1, Elham Yasari1, Nafiseh Farhadian1\* and Kourosh Malek2

1Chemicl Engineering Department, Faculty of Engineering, Ferdowsi University of Mashhad, I. R. Iran.

2Institute of Energy and Climate Research, IEK-13: Theory and Computation of Energy Materials, Forschungszentrum Jülich, 52425 Jülich, Germany

\*Corresponding Author Email: n.farhadian@um.ac.ir, Tel:+985138805140, Postal Code:9177948974

**Abstract**

Fine tuning the key performance indicators of a proton exchange membrane fuel cell (PEMFC) is computationally expensive and highly time-consuming due to nonlinear nature of the underlying physical phenomena. Here, artificial neural network (ANN) is applied to introduce a framework for PEMFC performance prediction composed of various catalyst layers based on experimental data. Carbon-based cathode materials such as reduced graphene oxide (rGO), graphene oxide (GO), graphene nanoplatelets (GNP), and carbon black (CB) and their hybrid including various Pt catalyst content are examined. Total surface area of the cathode and Pt content are selected as input variables, whereas electrochemically active surface area (ECSA), cyclic voltammetry diagrams, and current density-voltage-current power diagram are selected as output ANN responses. In this framework, experimental data for various cathode materials are initially classified using support vector machine and ANN models are applied to predict the performances. Results indicate that data are well classified into four main groups including Pt, rGO-CB-Pt, CB-Pt, GNP-CB-Pt, so that an ANN can achieve the best prediction performance with mean squared error less than 0.3% and relative error of 0.5%. Indeed, ANN application can be proposed as a useful tool for prediction the performance of PEMFC in comparison to experimental studies.

**Key words:** PEM fuel cell; Carbon-based cathode; Artificial neural network (ANN); Support vector machine; Cyclic voltammetry; Power density.

1. **Introduction**

Fuel cell technology is a mature and established electrochemical conversion system that generates high-efficiency electrical energy from the direct combination of fuels such as hydrogen and oxidizer such as air without causing environmental and noise pollution [1-4]. One of the most widely used fuel cells for automotive applications due to their high energy density and low operating temperature are Proton Exchange Membrane Fuel Cells (PEMFCs). In the anode of PEMFC, hydrogen atoms are ionized to electrons and proton (H+). Protons then penetrate the surface of the porous proton conducting membrane, usually a polymer electrolyte membrane (PEM) and move towards the cathode. Electricity is generated, since electrons cannot pass through the membrane and instead pass through an external circuit. In the cathodes, electrons combine with protons and oxygen in the air to form water [5]. The reaction in the anode is relatively slow and very slow in the cathode, so the platinum (Pt) catalyst is used on two levels of the electrolyte membrane. Recently, platinum nanoparticles are used as the catalyst for the electrochemical reactions at the anode and cathode due to high surface area toward weight ratios which reducing the amount of the costly platinum. Other parameters that affect the performance of the PEMFC include total surface area of the cathode and electrochemical active surface area (ECSA). Each catalyst layer type has a unique cyclic voltammetry diagram and current density-voltage-power density based on the cathode material type, catalyst type and content, membrane type, operating pressure and temperature. Among various types of cathode materials, carbon-based materials such as graphene oxide (GO) [6], reduced graphene oxide (rGO) [7,8], graphene nanoplatelets (GNP) [9], carbon black (CB) [7-9], ketjen black and Vulcan [10,11] are very common [12]. Recently, hybrid of these carbon-based materials have been applied as a support for Pt catalyst. In addition, applying these supports together with various ratios as hybrid materials exhibits different performance [12]. For example, Brian Seger and Prashant V. Kamat used graphene oxide as a support material for Pt nanoparticles dispersion for application in PEM fuel cells [6]. Nearly 80% enhancement in the ECSA obtained by exposing partially GO-Pt films to the main graphene support [6]. In addition, Ayse Bayrakceken Yurtcan and Elif Das. synthesized hybrid rGO and commercial CB in various weight ratios (rGO to CB weight ratios changed from 90:10 to 50:50) as Pt support. Their results showed that hybrid cathode material with the weight ratio of 70:30 (rGO:CB) has the best PEMFC performance [7]. Hybrid support materials were also applied to catalyst layer, consisting of CB and GNPs with different percentages for loading Pt nanoparticles. Results showed that hybrid material with 60% GNP has the highest PEMFC performance [9]. Accounting for these recent experimental studies, one may conclude that hybrid cathode materials due to their significant properties, they can contribute to the excellent performance of fuel cells and are a suitable candida for application in PEMFCs. However, available experimental results confirm that there is not a linear trend among ratios of the hybrid carbon materials and fuel cell performance from ECSA and power density point of view [12]. Also, performing experimental studies with various cathode types and different material ratios is highly labor intensive and time consuming. So, modeling the performance of PEMFC by emphasizing the cathode materials type can be very useful. Mathematical modeling has the capacity of synthesizing complex materials and investigating transport phenomena inside them, is inexpensive, rapid and robustness. To the best of our knowledge, there has not been any systematic computational and modeling studies of hybrid cathode materials for PEMFCs especially prediction the cyclic voltammetry diagrams with nonlinear phenomena.

Here, for the first time, we classified various hybrid carbon based materials as PEMFC cathode versus different properties by applying available experimental data. Then, artificial neural network (ANN) as a suitable machine learning (ML) tool was applied to predict the performance of PEMFC for various catalyst layer. Complicated and nonlinear diagrams of cyclic voltammetry and current density-voltage-power density for each catalyst layer type based on the cathode material was plotted and compared with available experimental data. Finally, a unique data-driven framework which predict the class of data and voltammetry diagrams were introduced.

**2. Mathematical Modeling**

A framework including the cathode material classification (level 1), artificial neural network modeling (level 2) and ECSA calculation (level 3) has been proposed in Figure 1. Each of these levels are introduced in details in the following sections.

**Figure 1. ANN modeling Framework**

**2.1 Data Classification**

First, all available experimental data based on PEMFC which apply carbon based cathode materials were gathered. All related properties of cathode materials such as cathode components as hybrid material, total surface area, Pt catalyst percentage are reported, too. Results are shown in supporting file (Table S1). Each experimental data that had complete cathode properties with defined cyclic voltammetry and density current- voltage- density power diagrams were selected for data classification (Table 1). By applying Table 1, cathode materials were classified into four main groups, including platinum (Pt), rGO-CB-Pt, CB-Pt, GNP-CB-Pt. Furthermore, each of hybrid cathode materials were divided into several subgroups based on the weight percentage of their components (Table 2).

**Table 1. Final data classification for cathode materials of PEMFC based on experimental data.**

**Table 2. Classification of cathode materials based on weight percentage.**

Then, in order to select features, some important properties (features) of cathode materials were investigated for classification of various groups. These features were total surface area, Pt percentage, Pt nanoparticle diameter. The results of this part have been discussed further in section 3.1.

**2.2. Artificial Neural Network Modeling**

In order to framework, artificial neural network (ANN) was applied to obtain cyclic voltammetry and current density-voltage-power density diagrams based on available experimental data. One of the most powerful methods for modeling processes in which the relationship between variables is nonlinear and complex is the ANN method.One of the advantages of ANN is that it can provide a nonlinear model between inputs and outputs with appropriate accuracy without the need for basic process information. This model can later be used to calculate the output of other inputs [13].

To create a model, an input and output data set must first be created. Based on the available graphs in previous experimental studies (Table 1), all the information related to the graphs was received for each cathode type and used as input in modeling. Then, the cyclic voltammetry data normalized between -1 and +1 by applying equation (1) in which they include positive and negative values. In addition, equation (2) was applied for current density-voltage-power density data to convert them to the normal values ​​between 0 and 1 because they are positive values [13].

y= $\frac{2x-(max+min)}{max-min}$ (1)

y=$\frac{x-min}{max-min}$ (2)

Here, the normalized value of 𝑥 is defined as 𝑦, besides, the maximum and minimum values of 𝑥 are summarized as 𝑚𝑎𝑥 and 𝑚𝑖𝑛, respectively.

In the current study for training, validation and testing neural network models, 70% , 15% and 15% of the data were used, respectively. Random selection of sets to decrease the impact of data order on ANN performance is detrimental and has been considered in the current study. Multilayer perceptron (MLP) is one of the interesting ANN structures with appropriate performance in many applications [14-17]. It composed of three layers: input, hidden and output. In this structure, number of neurons in the first and third layers is equal to the variables number in inputs and outputs of the model. Moreover, ability of estimation of the model, complexity and possibility of overfitting have been affected and controlled by the number of hidden layers, the more the hidden layers the more the possibility of aforementioned are. Basically, a neural network with a hidden layer and a sufficient number of neurons in this layer can have an acceptable prediction of the relationship between inputs and outputs [18,19].

A three-layer ANN structure is composed of a hidden layer and has been proposed to work well in many studies [14, 20-24]. In addition, neural network with two hidden layers has also been reported in some papers [15, 16, 25, 26].

In order to optimize the structure of the ANN and determining the number of hidden layers, trial and error method is used. The performance and ability of each structures for estimation then are compared.

 The mean square error (MSE) is used as a performance index to choose the optimal ANN code. The mathematical equation of this parameter is as equation (3) [20]:

MSE= $\frac{1}{N}$ $\sum\_{i=1}^{N}(Yexp,ᵢ-Ypred,ᵢ)²$ (3)

Here, 𝑌exp,i is the experiment value , 𝑌𝑃𝑟𝑒𝑑,i is the prediction value and N is the number of input-output data of the set.

Besides, the bias and correlation (R) parameters are also examined. These two parameters demonstrate the performance of the optimal model better. Bias is defined as the mean of the difference between the predicted value and the experimental values (obtained from the literature). Bias parameter is defined as equation (4) [20].

Bias= $\frac{\sum\_{i=1}^{N}(Yexp,ᵢ-Ypred,ᵢ)}{N}$ (4)

Where, 𝑌exp,i is the actual value, 𝑌p𝑟𝑒𝑑,i is the predicted value by the model and 𝑁 is the number of data,.

Correlation coefficient is a numerical measurement of a kind of correlation, meaning a statistical relationship between two variables. It defines the intensity as well as relationship type such as direct or inverse. The value of this coefficient may vary between 1 and -1. It is equal to zero when there is no relationship between two variables. The correlation between X and Y as two random variables is defined as shown in equation (5) [13].

Corr(X,Y)= $\frac{cov(X,Y)}{σX σY}$ (5)

Where cov means covariance, corr is the usual symbol for correlation and σ is the standard deviation symbol.

Here, a feed forward MLP was used as ANN model with the sigmoid transfer function (𝑓1=𝑠𝑖𝑔) in the hidden layer(s) and the linear transfer function (𝑓2=𝑝𝑢𝑟𝑒𝑙𝑖𝑛) in the output layer. The most important elements of neural networks are neuron which are located in the hidden and output layer as was mentioned earlier. Equations (6) and (7) are shown the mathematical formulation of neurons in hidden and output layers:

 *ai=* $\sum\_{i=1}^{m}Wᵢᵧ Xᵧ$ (6)

*ni= f (ai + bi)* (7)

where, input values to the neurons are defined as 𝑋ᵧs, the the i-th neuron weights regarding to the j-th input are defined as 𝑊ᵢᵧs, bias value of the i-th neuron is 𝑏i, f(-) is the activity function, and last but not least 𝑛i is the output value of the i-th neuron. Outputs responses are estimated by equation (8):

Output= f2 (WO\* f1 (WH\* X+ bH) + bO) (8)

Here, 𝑊H and 𝑏H are the weights and biases of the hidden layer and 𝑊O and 𝑏O are weights and biases of output layers, respectively.

Levenberg-Marquardt Back Propagation (BP) algorithm is used for training. In BP algorithm, the error between the experimental and predicted data is continuously returned to the network to be minimized. Weights are adjusted to minimize this error. Weight changes continue to provide convergence conditions such as the number of iterations or the minimum error and so on. In the current study, the stopping criterion for the training phase was set to 1000 iteration. Besides, in order to prevent overfitting, when an increase of MSE of the validation data parallel to a decrease or stagnation of training data happened in a 6 consecutive epoch the training phase is stopped and the minimum MSE of the training data are used as the best network weights.

Finally, among the studied structures of neural networks, the structure with the minimum of total MSE (defined for the training, validation and testing subsets) was determined as the optimal structure. It should be noted that all modeling was performed using ANN tool box which is implemented in MATLAB 2017 Software.

Here, two types of data modeling were performed: In the first modeling, to achieve cyclic voltammetry diagram, total surface area, Pt percentage and voltage were determined as inputs and the current was selected as the output. In the second modeling, to achieve current density-voltage-power density diagrams, total surface area, Pt percentage and current density were selected as input. Voltage and power density were selected as output. Both types of modeling were performed separately for each group. After calculating the cyclic voltammetry diagram, ECSA value was calculated using equation (9). In this equation, QH is the total charge for hydrogen ion excretion that is calculated the integral of the area under the hydrogen ion excretion diagram (H+) in the CV diagram [8].

ECSA [cm2Pt ⁄ g­Pt]= $\frac{charge\left[QH,\frac{μC}{cm2}\right]}{210\left[\frac{μC}{cm2}\right]\* electrode loading\left[g\frac{Pt}{cm2}\right]}$ (9)

Here, the value of QH is calculated using the trapezoidal method to calculate the integral of the area under the hydrogen ion excretion diagram (H+) in the CV diagram.

**3. Results and Discussion**

**3.1 Data classification**

The classification diagrams based on these properties are shown in Figure 2. As Figure 2 shows each diagram that could separate groups from each other can be useful (framework level 1). Among various diagrams, only Pt percentage versus total surface area is suitable for this aim.

**Figure 2. Data classification diagram for different cathodes based on the (a) Pt nanoparticle size and Pt percentage, (b) total surface area and Pt nanoparticle size and (c) total surface area and Pt weight percentage.**

Then, data classification was performed using MATLAB software classification toolbox by applying various methods such as Cosin k- nearest neighbors’ algorithms of support vector machines including linear, quadratic, cubic, fine guassian, medium guassian and coarse guassian and fine-medium-coarse decision tree algorithm. After training a model in Classification Learner, the best overall accuracy in percent was obtained for the model SVM-cubic (Table 3). So, it was selected as the final model for predicting the group to which unknown cathode belongs. Also, the prediction diagram and confusion matrix of SVM-cubic method for different cathodes are shown in Figure 3, respectively. According to confusion matrix the accuracy for class 2, 3 and 4 is 86%, 67% and 100%, respectively.

Now, according to Figure 1 (framework level 2) by entering two values of the total surface area and Pt percentage in the unknown cathode and implementing the SVM-cubic model, the group to which the cathode belongs is determined.

**Figure 3. (a) Prediction diagram of SVM-cubic method for different cathode, (b) Confusion matrix SVM-cubic method for different cathode.**

**Table 3. Accuracy of different classification methods.**

In the next step, accuracy of ANN model was examined by computing MSE, R, Bias and weight matrices versus various neurons number for the first and second modeling. Results of MSE and R are shown in Table 4. Other parameters are reported in supporting file (Tables S2-S4).

**Table 4. Modeling parameters for cyclic voltammetry diagrams (first modeling) and current density-voltage-power density diagrams (second modeling)**

As it was shown, the values of mean least square error for all models are less than 0.3%, which is an acceptable result. Also, the value of R for all cases is more than 0.995, which shows a good correlation between the experimental and predicted data. From the values of these two parameters, it can be concluded that the obtained models can well predict the desired graphs.

After accessing the desired models, to ensure the accuracy of the modeling, both types of modeling were performed (framework level 3) for the training data. Figures S1-S4 (supporting file) show a comparison between the experimental data and the values obtained from the modeling.

As mentioned earlier, initially 15% of the experimental data were separated from each of the graphs for validation and now with the implementation of this data in both types of modeling, we can confident the accuracy of the model. These diagrams are shown in Figures S5-S8.

Also, in both of modeling, 4 of the 16 graphs were initially excluded for testing, by entering this data in the models and executing the program, we can evaluate the performance of both models. Figures 4 and 5 show results. As can be seen from the graphs, the models were able to predict the graphs well. Therefore, it is possible to ensure the performance of the models and use them in similar cases.

**Figure 4. Cyclic voltammetry diagrams with test data for a) rGO-CB (H90-H60), b) GNP-CB (H90-H70) cathodes.**

**Figure 5. Current density-voltage-power density diagrams with test data for a) rGO-CB (H90-H60), b) GNP-CB(H90-H70) cathodes.**

In Table 5, the calculated and experimental ECSA values are compared to each other. As can be seen, the error value obtained for all groups is less than 5% and the average error for the GNP-CB group has the lowest value. This indicates the acceptable accuracy of the model for prediction the data.

**Table 5. Comparison of the calculated and experimental ECSA values.**

Finally, by running the program, the user asked to inter the total surface area of the material (m2/g) and the percentage of Pt (wt%) in the cathode. Then, in the classification level, the materials are executed first and the group to which the unknown cathode belongs is specified. After that, the first model is executed and the cyclic voltammetry diagram is obtained. Next, obtaining the cyclic voltammetry diagram, with the help of hydrogen ion excretion diagram, the ECSA value is calculated and by performing the second modeling program, the current density-voltage-power density diagram is obtained. By applying the program, it will be possible to get all necessary data for an unknown cathode material based on carbon. Also, with the help of current density-voltage-power density diagram, the maximum production power versus different voltage can be evaluated.

**4. Conclusion**

In this study, cyclic voltammetry and current density-voltage-current power curves of a proton exchange membrane fuel cell has been predicted by introducing a unique data-driven framework applying artificial neural network modeling using available experimental data. Carbon based cathode materials such as graphene oxide (GO), reduced graphene oxide (rGO), graphene nanoplatelets (GNP) and carbon black (CB) as well as their hybrid materials were selected for this aim. Important parameters of cathode materials such as total surface area, Pt catalyst weight percentage were assumed for data classification by analyzing different features. The results obtained from data classification showed that SVM cubic method with 87.5% accuracy is the best one for prediction the cathode class. Furthermore, results of the modeling show that ANN with 3 layers and between 2-24 neurons could accurately predicts the training, validation and test data. Comparing the calculated ECSA value of the modeling with the experimental results showed that the model can well calculate the ECSA value, so that the error value obtained for all groups is less than 5%. All results confirmed that the proposed framework based on ANN can be a suitable ML tool for predicting the complicated and nonlinear behavior of PEMFC behavior in which it can be applied for other types of cathode materials in the same or different types of fuel cells.

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