

# Application of artificial neural network in performance prediction of PEM fuel cell<sup>‡</sup>

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## SUMMARY

Investigations on using artificial neural networks to predict the performance of single proton exchange membrane fuel cell has been carried out. Two sets of polarization data obtained at different temperatures and flow rates are used to create and simulate the network. Cell temperature, humidification temperatures, H<sub>2</sub>/air flow rates and current density have been used as inputs, and voltage is used as observed (output) value to train and simulate the network. This nonlinear data are batch trained, and artificial neural network has been constructed using feed forward backpropagation algorithm. Performance of the training has been improved by increasing the number of neurons to reduce the error. Simulation results are in agreement with experimental data, and the corresponding networks are used to predict the polarization behavior for unknown inputs. Copyright © 2011 John Wiley & Sons, Ltd.

## KEY WORDS

PEMFC; ANN; FFBP; fuel cell

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## 1. INTRODUCTION

Polymer electrolyte membrane fuel cell, a low-temperature fuel cell, is being increasingly evaluated in various applications owing to the simplicity of its construction, modular nature, quick start-up, and higher efficiency. Performance improvement, size reduction, durability, and cost reduction are some of the major research and development activities in recent times to place these devices firmly in various application domains. Improvement in the performance is addressed on several fronts, viz. new materials with improved characteristics, minimizing the losses in the fuel cells especially the ohmic losses in the cell assembly, and so forth [1]. These studies are laborious because they involve investigating a wide variety of parameters such as the properties of the materials used, method of preparation, different combinations of the materials used, and operating conditions such as humidification temperature, cell temperature, flow rates of the reactants, pressure, and so forth, allowing for several permutation and combinations.

Mathematical models are helpful tools for the design and optimization of fuel cells performance and help in reducing the number of experiments to be carried out. Many physical models have been developed to examine the complicated transport and electrochemical phenomena in hydrogen-fed proton exchange membrane (PEM) fuel cells [2–7]. Unfortunately, several of these physical models are not sufficient to arrive at a relationship between the input and output variables to predict the fuel cell performance under different conditions. Artificial neural network (ANN) model provides useful and reasonably accurate input–output relations because of its excellent multidimensional mapping capability [8,9]. Using this simulation method, we can simulate the behavior of PEM fuel cell under different conditions. Vicky *et al.* [10] proposed a NN modeling approach for the mechanical nonlinear behavior of a PEM fuel cell system in which a fuel cell system in operation is subjected to random and swept-sine excitations on a vibrating platform in three axes directions by using a multilayer perceptron NN and in which good accuracy with the

experimental results was achieved. They suggested that this approach, in a real-time system, provides an environment to analyze the performance and optimize the mechanical parameters design of the PEM fuel system. And also, many issues that affect the performance of the fuel cells can be diagnosed using this simulation method. Steiner *et al.* [11] have used ANN for diagnosing the faults in the fuel cell system. Their diagnosis procedure of water management issues in fuel cell, namely flooding and drying out, is based on a limited number of parameters that are, besides, easy to monitor. This group employed a procedure called black-box model based on NNs that simulates, in case of healthy operation, the evolution of pressure drop at the cathode as well as the fuel cell voltage. This analysis permits the detection and the classification of fuel cell's states of health between flooding, drying out, or normal operation. Also, Kumbur *et al.* [12] have developed a diffusion media (DM) design tool using ANN for multivariate optimization of multiphase transport in fuel cell DM. This study explores the development of a DM design algorithm based on ANN that can be used as a powerful tool for predicting the capillary transport characteristics of fuel cell design media. In such a way, the performance of the fuel cells can be predicted under different conditions.

An ANN is a computational method that interconnects inputs and outputs with the help of processing units known as 'neurons'. This computational method has recognition in many areas of science and technology such as pattern recognition, signal processing, and process control in engineering [13]. Although statistical regression analysis, another mathematical model, can be used for prediction problems, it has some limitations on the input data, viz. highly correlated data in the input cannot make a good relation with the output. Under these circumstances, ANN appears to be a suitable alternative for the prediction problems. In 2008, Ernis [14] has focused on the heat transfer analysis of compact heat exchangers through ANN. The trained ANN results perform well in predicting the heat transfer coefficient, pressure drop, and Nusselt number with an average absolute mean relative error of less than 6% compared with the experimental results. Also, Tien *et al.* [15] have carried out prediction studies on the hydrogen safety parameters using ANN. A predictive model for accurate estimation of hydrogen parameters such as percentage lower explosive limit, hydrogen pressure, and hydrogen flow rate as a function of different input conditions of power supplied (voltage and current), the feed of de-ionized water, and various parameters is carried out in their work. The explosive limits of hydrogen were predicted to be  $\pm 2\%$ , the  $H_2$  pressure and flow rates were predicted to be  $\pm 5\%$  and  $3\%$ , respectively. They have compared the network prediction results with its actual output target values, acquired from expensive sensors, which are extremely close. So, using this kind of simulation methods can avoid not only the number of the experiments but also the use of expensive instruments. In recent times, the performance prediction of single fuel cell or fuel cell stack using ANN has appeared in literature. Bhoopal *et al.* have investigated the performance of 18-watt fuel cells

using backpropagation (BP) algorithm with just hydrogen pressure and stack current as the two input variables. From their simulation results, they concluded that a BP-based NN can successfully predict the stack voltage and the stack current of a PEM fuel cell stack [16,17]. The selection of the number of neurons for relating the input and output parameters also plays a major role in this simulation. If the number of neurons is more, the relation between the input and the output will be complex, and the network formed with this relation will not be suitable for proper prediction. Saengrungs *et al.* [18] have studied the performance prediction of a PEM fuel cell stack using ANN with two inputs and two outputs with three hidden layers. They investigated various network architectures by varying the number of neurons and hidden layers to determine which one tends to give a faster and better prediction performance. From their observations, they concluded that even the BP network with one hidden layer of 3 or 10 neurons can provide a good prediction in terms of speed and accuracy. These results concluded that a more complicated network may not necessarily perform better than a simpler one.

So, the aforementioned studies are carried out either by using multiple hidden layers using more neurons or by using less number of input parameters with high neuron number. Our aim in this study is to use less number of neurons with single hidden layer by using more number of input parameters and also to reduce the number of experiments using ANN. Initially, the predicted performance was confirmed with experimental data. Finally, the prediction of performance in regions of temperature where experiments were not performed has been carried out. In the first part of this paper, the statistical regression analysis and the ANN model construction are described briefly. In the second part, how this model has been successfully used in our studies to predict cell performance of fuel cells developed in our laboratory is presented.

### 1.1. Statistical regression analysis

Statistical regression analysis has been often used for prediction problems. Regression analysis for studying more than two variables at a time is known as multiple regressions. The multiple linear regression models take the following form:

$$Y_i = b_1 X_{i1} + b_2 X_{i2} + \dots + b_k X_{ik} + e \quad \forall i = 1, 2, \dots, n \quad (1)$$

In simplified form, it is written as

$$Y = Xb + e \quad (2)$$

where  $X$  is an input vector,  $Y$  is the vector of desired output,  $b$  is the vector of regression coefficients, and  $e$  is the vector of residual errors.

The least square coefficients are estimated by choosing  $b$  so as to minimize the sum of squared residuals  $e'e$ . Thus,

$$\begin{aligned} S(b) &= e'e = (Y - Xb)'(Y - Xb) \\ &= Y'Y - 2(Y'X)b + b'X'Xb \end{aligned}$$

Taking the derivative with respect to  $\mathbf{b}$  gives

$$\partial S(\mathbf{b})/\partial \mathbf{b} = 0 - 2\mathbf{X}'\mathbf{Y} + 2\mathbf{X}'\mathbf{X}\mathbf{b}$$

Setting this equal to zero,

$$\mathbf{b}_s = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} \quad (3)$$

However, there are some limitations on using the statistical analysis. When the data are more correlated, it is difficult to obtain a relation between the input and the outputs with minimum least square error.

## 1.2. Artificial neural network (ANN)

An ANN is a biologically inspired approach for problem solving. It is helpful for the applications where format analysis would be difficult such as pattern recognition and nonlinear identification. Like a biological neural system, an ANN can learn and be trained to find solutions, recognition of patterns, and predict future events. Artificial neurons make relation between the given input and output data. ANN provides a paradigm for solving problems whose output result is unknown and uncertain. The behavior of the ANN is defined by the way its individual computing elements are connected and by the strength of those connection and weights. Figure 1 shows a schematic representation of a single-neuron ANN system. Here,  $x_1, x_2, x_3 \dots x_n$  represents the input variables at the neuron; the formal neuron corresponds to the incoming activity of the biological neuron; and  $w_{1k}, w_{2k} \dots w_{nk}$  are the weight vectors representing the effective magnitude of information transmission between neurons, which are updated repeatedly during the training process.

Every input is combined with a weight at the input layer and given as an input to the combiner. The combiner makes an input relation for the given inputs. Later, the transfer function determines the behavior of the input and the output and forms a relation between them. The most significant difference between ANN and statistical modeling is the method used to derive the functional model. In statistical methods, the predefined models are tested on data sets, and then, a suitable model that will give the best

solution is selected. Developing an ANN involves preparing data for constructing a network, selecting a training algorithm (the learning rule), configuring the initial layout of neurons (the network architecture), and then monitoring training progress until a satisfactory model converges. This is always an iterative process in which results from successive training cycles inform modifications to the network or the training regime while repeating the process.

## 1.3. ANN algorithm

Artificial neural network algorithms can be defined to alter the connections between the layers and therefore processing to form a better network. Feed forward backpropagation (FFBP) algorithm is used for problems that have nonlinear data. The BP algorithm for training ANN was popularized by Rumelhart *et al.* [19] in 1986. In feed forward (FF) architectures, the activations of the input units are set and then propagated through the network until the values of the output units are determined. The network acts as a vector-valued function, taking one vector on the input and returning another vector on the output. The network is trained to give a better performance and to minimize the least square error function.

The error function is defined as

$$E = 1/2 \sum_{i=1}^k (t_i - O_i)^2 \quad (4)$$

where  $t_i$  is the desired target value associated with the  $i$ -th input data,  $O_i$  is the output of network when the  $i$ -th input pattern is presented to network, and  $k$  is the number of data points. To train the network, we adjust the weights in the network so as to decrease the error. This is called gradient descent and is defined as

$$\Delta w = -\eta \partial E / \partial w \quad (5)$$

where  $\eta$  is the learning rate,  $E$  is the error function,  $w$  is the weight, and  $\Delta w$  is the difference between the new and old weights. Weights keep modifying during the time of training process until the error is minimized. This can be achieved by trial and error method by changing the

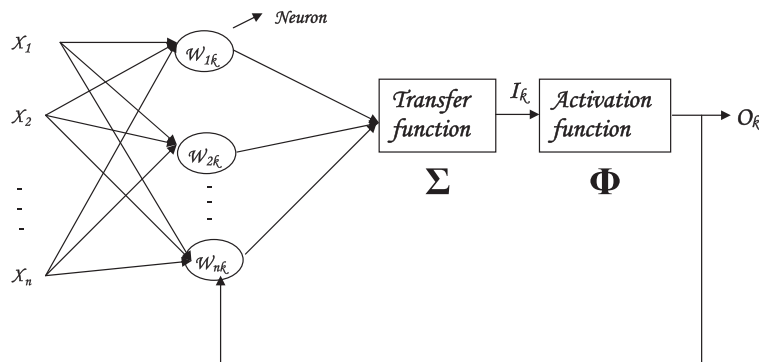


Figure 1. Schematic model for NN.

number of neurons. NN thus formed with minimal error is ready to simulate the data. This network will make a powerful mathematical relationship of the dynamic system based on the input–output data.

## 2. EXPERIMENTAL

### 2.1. Fuel cell preparation

A PEM fuel cell consisting of a membrane electrode assembly with 5 cm<sup>2</sup> electrodes made by a proprietary Centre for Fuel Cell Technology process [20] where 40% Pt/C with 0.25 mg cm<sup>-2</sup> loading is used as an anode catalyst and 15% Ce<sub>0.8</sub>Zr<sub>0.2</sub>O<sub>2</sub>–40% Pt/C with 1 mg cm<sup>-2</sup> loading is used as cathode catalyst and Nafion membrane (212) as electrolyte. The membrane electrode assembly is placed between the graphite flow fields and current-collecting copper plates. The cell is finally tightened using end plates. The cell was tested in ARBIN (MITS pro FCTS model, Arbin instruments, Texas, U.S.A.) fuel cell test station under various conditions of cell temperature, humidification temperatures, and flow rates of hydrogen and air. Hereafter, the humidification temperatures and cell temperatures are denoted as  $T_{H_2}/T_{cell}/T_{air}$  and hydrogen, air flow rates as  $H_2/air$ . Polarization data (voltage–current density curves) were then generated for the single fuel cell.

### 2.2. Simulation

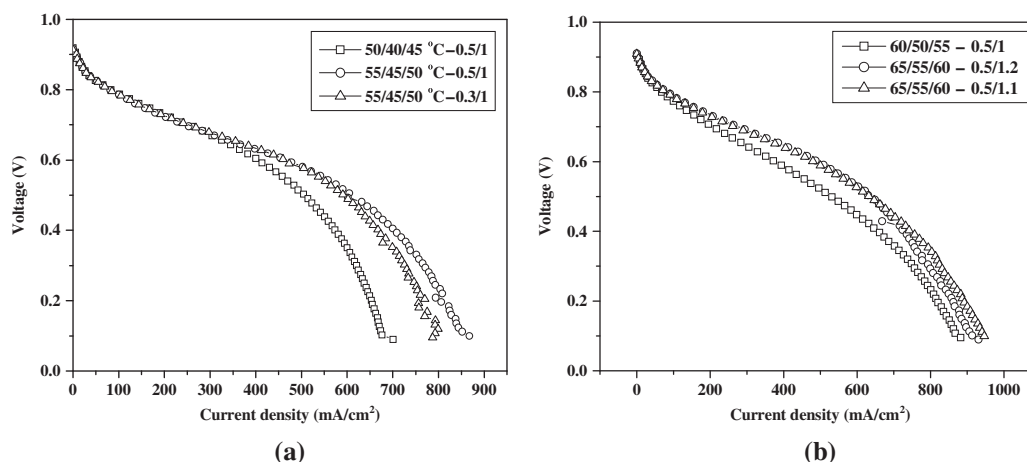
An ANN simulation was utilized to predict the performance of the PEM fuel cell with the help of Matlab R2007b (MathWorks Inc., Natick, MA) software. For these predictions, the data from the experiments performed on the fuel cell were used to form the network using backpropagation algorithm, and the data were batch trained by varying number of neurons to minimize the least mean square error. Using this network analysis, we carried out the simulation at different temperatures with different flow rates and compared

the performance with the experimental. Also, performance prediction has been carried out for unknown cell temperatures and flow rates.

## 3. RESULTS AND DISCUSSION

### 3.1. Experimental results

The experimental data that are generated are used to train and test the polarization curves at different temperatures and flow rates. PEM fuel cell prediction was carried out at different flow rates of reactants for different temperatures (data set a) and different temperatures at constant flow rates (data set b). Figure 2 shows the polarization curves of the first set of data (data set a). In this, the fuel cell performance data operated at the temperature range of 40–55 °C at different  $H_2/air$  flow rate conditions were used to train the network. The total number of experimental data taken for training the network was six. Figure 2a shows the polarization curves of fuel cell between 40 and 45 °C at different flow rates. This plot reveals that the performance of the cell is improved at 45 °C under high flow rates, which can be seen from the higher current densities obtained at 0.6 V, which explains that with the increase of cell temperature, humidification temperatures, and flow rates, the performance of the cell increases. This has shown improvement in the mass flow region (at higher current densities) other than active and ohmic regions (lower current densities). Figure 2b shows the curves at 50 and 55 °C at different high flow rates. This plot shows that performance at higher current densities has increased for high temperature, humidification temperatures, and high flow rates compared with that of the low temperatures (at 40–45 °C). At these, high temperature improvement is observed in both active and mass flow regions (lower and high current densities). But the performance of the cell is slightly decreasing at very high flow rates of gases. So, it is concluded that with the increase of cell temperature,  $H_2/air$  humidification temperatures, and  $H_2/air$  flow rates, the performance of the cell increases. But if



**Figure 2.** Polarization curves of training data set (a) at 40, 45, and 50 °C at different  $H_2/air$  flow rates and (b) is at 50 and 55 °C at higher flow rates.

the flow rates are much higher, that leads to the decrease in the performance of the cell. So, optimized conditions are to be maintained for the improved fuel cell performance. The aforementioned six experimental data are used to train the NN, and trained network has been tested on other polarization curves data using the same input parameters that are used for training the aforementioned network; as shown in Figure 3 (testing-data curves), the output voltage obtained on testing this testing data with trained network is with the experimental results. Here, the number of input parameters is six current density,  $H_2$  and air flow rates,  $H_2$  and air humidification temperatures, and cell temperature. The aims of taking this set of data are to predict the performance of the fuel cell at different temperatures in the range of trained data temperatures with different flow rates other than the trained data and make comparison with the experimental data and to study the effect of the number of input parameters in training the network. All flow rates mentioned as  $H_2$ /air in the figures are in the units of liter per minute (lpm).

Figure 4a shows the second set of data at different temperatures with constant  $H_2$ /air flow rates (equal to 0.5/

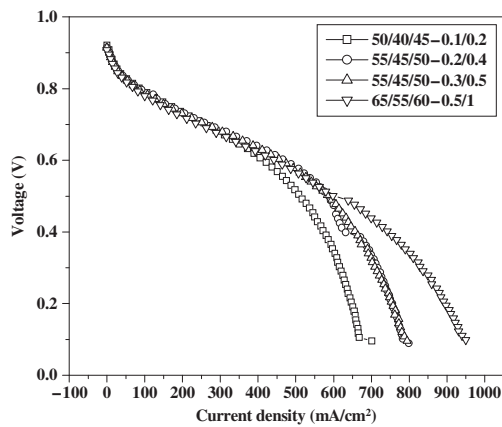


Figure 3. Polarization curves of testing data.

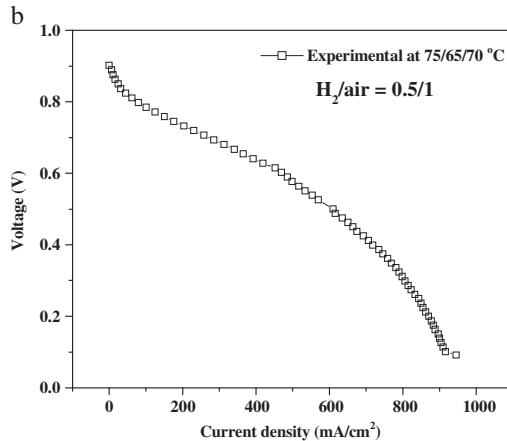
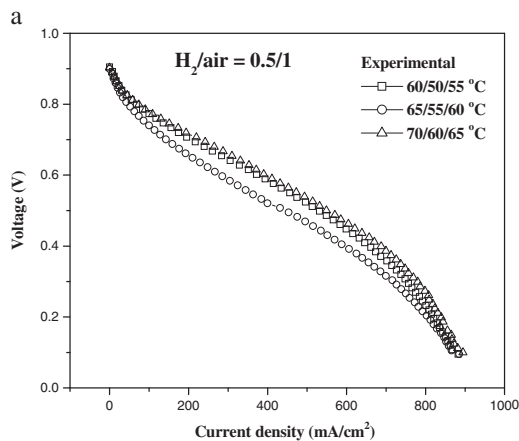


Figure 4. (a) Polarization curves of experimental training data set II at 50, 55, and 60 °C (b) testing data at 65 °C cell temperature with  $H_2$ /air flow rates equal to 0.5/1 lpm.

lpm). This plot shows that with an increase in the temperature, the performance of the cell is increasing in the active region. Here, the number of input parameters is four current density,  $H_2$  and air humidification temperatures, and cell temperature. The aims of this study are the same as those mentioned previously, that is, to study the effect of number of input parameters on NN and to predict the performance of the cell at unknown higher temperatures at same flow rates. Figure 4b is the testing data used to test the network at cell temperature of 65 °C.

### 3.2. Simulation results

Using the aforementioned set of experimental results, we simulated and predicted the polarization curves at different temperatures and flow rates. Network formed with the first set of data contains cell temperature,  $H_2$  humidification temperature, air humidification temperature,  $H_2$  flow rate, air flow rate, and current density as the input variables, and voltage as the output value. Figure 5 shows the schematic representation of the ANN used in the analysis of the present problem. Prediction problem was initially carried out using statistical regression analysis. Figure 6 shows the scattering plot of the first data set input variables to show the correlation between the variables. The closer the data points come when plotted to making a straight line, the higher the correlation between the two variables. Thus, from the scatter plot, it is ensured that the input variables are highly correlated. Because the input set is large and variables are highly correlated, the determinant of the matrix converges to zero. In such cases, it is not possible to compute the inverse of the matrix (to compute Equation 3, we need to find the inverse matrix  $(X'X)^{-1}$ ); hence, it is not possible to apply statistical regression techniques. The alternative for this problem is by using ANN. In ANN, it is presumed that the network that is trained with data at different temperatures with low and high flow rates is capable of predicting the polarization curves at other flow rate conditions within the trained data temperature range.

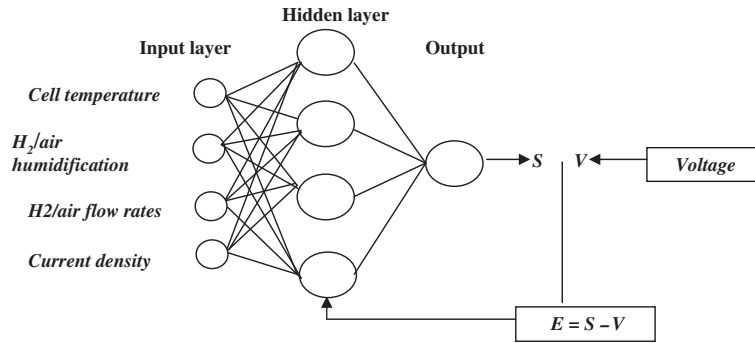


Figure 5. Schematic representation of backpropagation NN model.

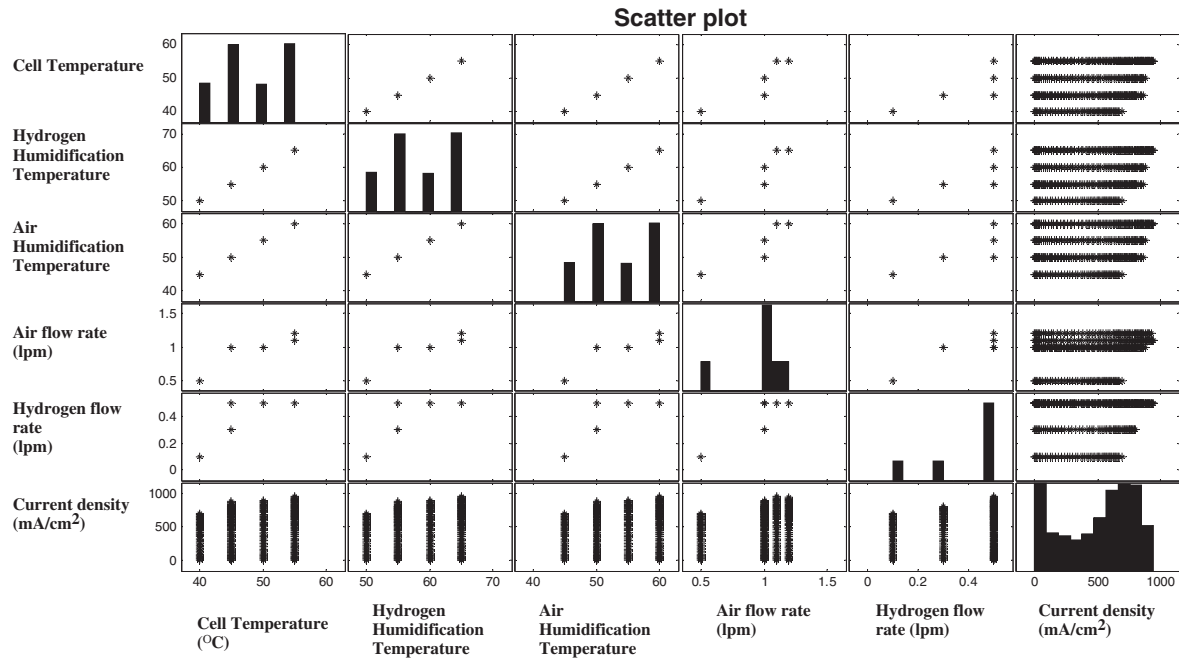


Figure 6. Scattering plot of the first set data input variables showing high correlation between each other.

Two-layered FFBP algorithm was used to train the experimental data. The number of neurons in the hidden layer was varied to predict the network performance. The number of neurons selected was four for the first data set, and the hidden layer was one. The transfer function selected for each layer was sigmoidal. Mean square error was then calculated for the desired output ( $S$ ) and experimental output ( $V$ ). Initially, the weights at the input of the hidden layer were selected randomly. If the calculated error between  $S$  and  $V$  is more, then the error between them becomes backpropagated and weights become modified until the error becomes less. Figure 7 is the learning error of BP algorithm for the first data set. The error performance was noted as 0.00013. Thus, the network was trained with the first set of data with minimal least square error. This trained network was initially tested to predict the data at low flow rate and low temperature.

Figure 8a shows the experimental and simulated curves at 40 °C with  $H_2$ /air flow rates equal to 0.1/0.2 lpm. From this plot, it is evident that the experimental and the predicted values are in agreement with each other. The same network was used to test the data at 45 °C at both low and high flow rate conditions. Figure 8b shows the experimental and simulated curves at 45 °C with  $H_2$ /air flow rate equal to 0.2/0.4 lpm, and Figure 8c shows the simulated and experimental curves at 45 °C with little higher flow rates at 0.3/0.5 lpm. In both plots, the experimental and the predicted curves are in agreement. Later, the same network was tested for further high temperature at 55 °C at higher flow rates equal to 0.5/1 lpm as shown in Figure 8d. This also confirms the good agreement between the experimental and predicted curves. So, the same network was used to make predictions at unknown flow rates. From all the four simulated results, it



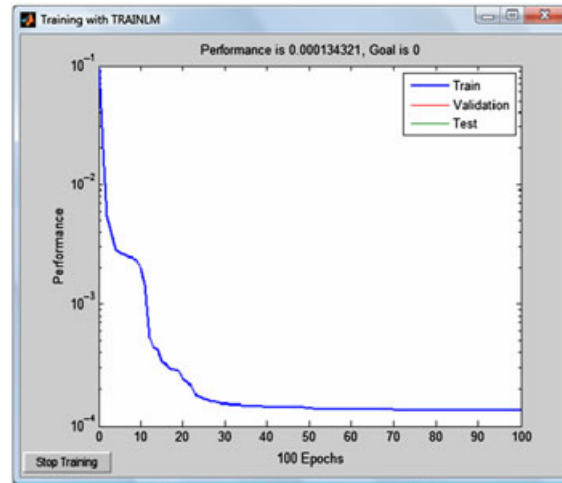


Figure 7. Learning error of backpropagation algorithm for the first set of data.

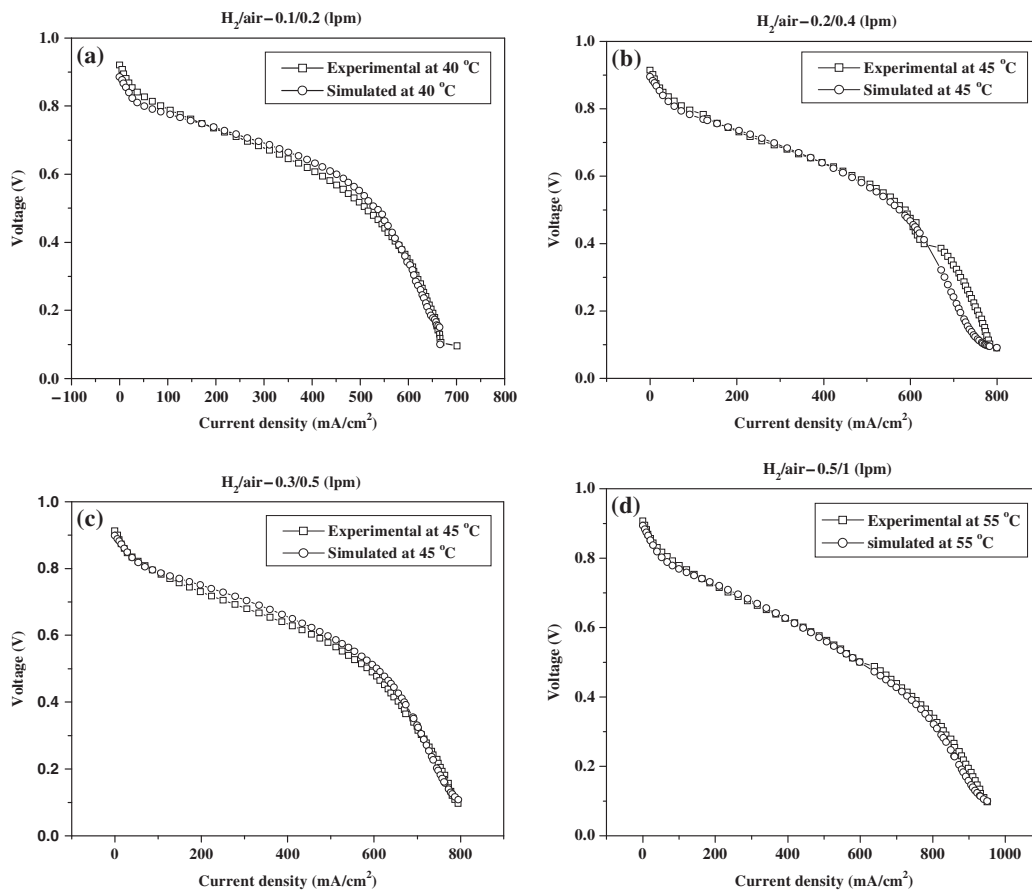
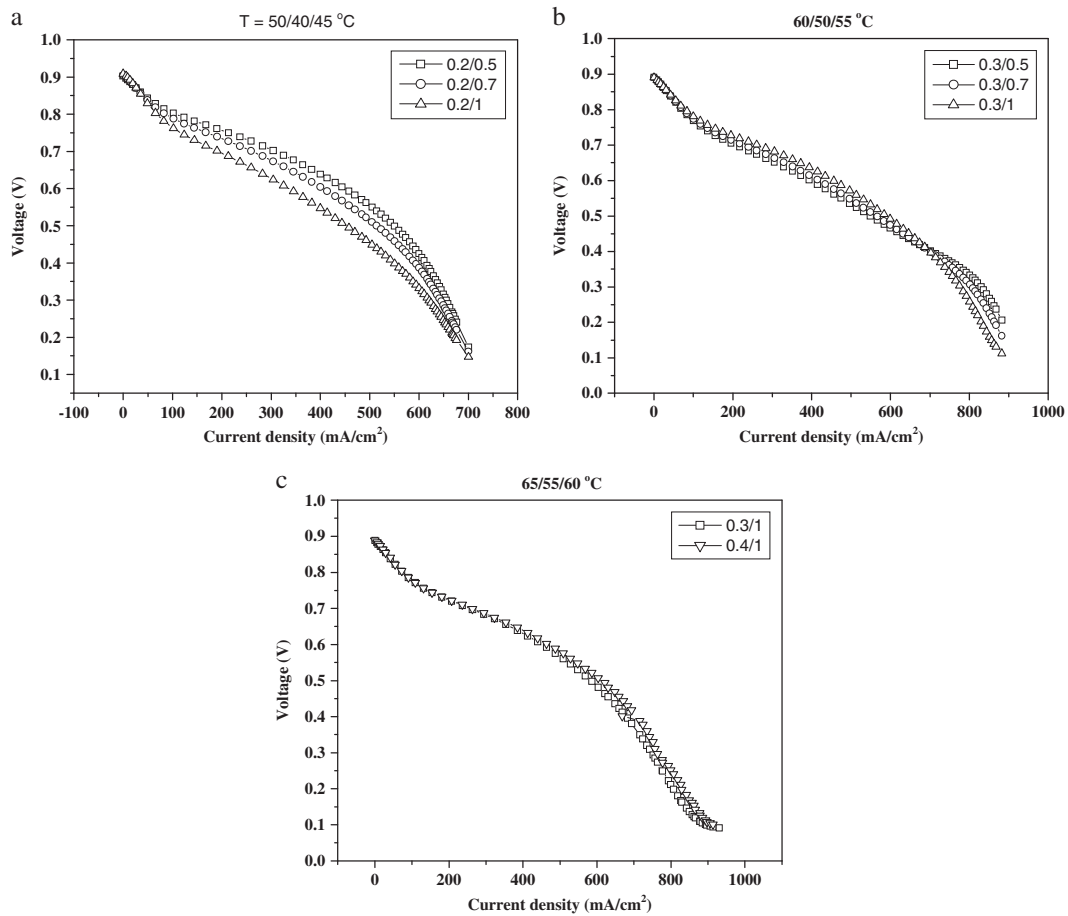


Figure 8. Comparison between the simulated and experimental data.

is noticed that with the increase of the temperatures from 40 °C to 55 °C, humidification temperatures, and flow rates, the performance of the cell is also increased in the simulated behavior following same trend as experimental.

Figure 9 shows the prediction plots carried out at different flow rates. Figure 9a shows the prediction plots at 40 °C at different flow rates. This plot explicates that at 40 °C, with an increase in the air flow rate, the performance of the cell is



**Figure 9.** Performance prediction plots of PEM fuel cell (a) at 40 °C (b) at 50 °C (c) 55 °C cell temperatures at different flow rates.

decreasing. As we can see, it ensures that to activate the catalyst sites of catalyst layer, optimum temperatures should be maintained. Figure 9b shows the performance prediction at 50 °C with different flow rates, and this plot shows the improvement in the ohmic region but not in the mass transfer region. Figure 9c shows the performance prediction at 55 °C. Here, with an increase in the flow rate, there is a slight increase in the performance observed. In this way, the performance of the cell has been predicted by varying different input variables with less number of experiments.

From these results, it can be inferred that the network trained with the data sets (at different temperatures with low and high flow rates) can be useful for predicting the performance at other flow rates within the temperature range of trained data. In the second set of data, cell temperature, H<sub>2</sub> and air humidification temperatures, and current density are taken as input parameters and voltage as the output values, and temperature range is 50–60 °C. The number of experimental data used for training is three. Here also, the statistical regression analysis failed to get a relation because of the high correlation between the inputs. The same two-layered FFBP algorithm and sigmoidal transfer function were used to train the network. The

number of hidden neurons was five, and the number of hidden layer was one.

During the training process, the error curve variation for the second data set is shown in Figure 10. Error obtained is minimal using the previously given algorithm and the number of neurons. Thus, the performance of the network meets the desired output. This trained network was used to simulate the response of voltage/current of the PEM fuel cell. First, this network was used to simulate the data at 65 °C and compared with the experimental voltage as shown in Table I. It can be seen that the simulated data are in reasonable agreement with the experimental data. In Figure 11, the polarization curves of the experimental data and the simulated data at 65 °C are compared. On condition of the same current density, improving the working temperature would lead to the increase of output voltage, which favors improvement of cell performance. The current density at 0.1 V is kept as 1000 and 1200 mA/cm<sup>2</sup> for 70 and 75 °C cell temperatures, and the performance predictions were carried out using the same network as that shown in Figure 12.

The polarization curves for the simulated data show improvement in the performance of the fuel cell in the ohmic region compared with the lower temperatures and a slight



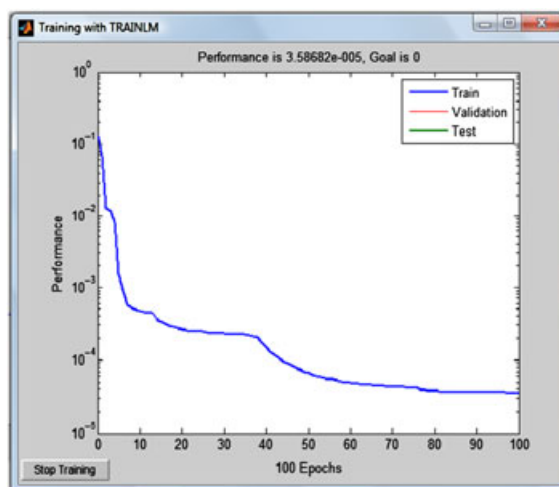


Figure 10. Learning error of backpropagation algorithm for the second data set.

Table I. Comparison between experimental and simulated voltages at 65 °C cell temperature.

Cell temperature (°C)	Current density (mA/cm <sup>2</sup> )	Experimental voltage (V) (out-put)	Simulated voltage (V) (out-put)
65	0	0.90208	0.8941
65	6.4953	0.88927	0.888
65	31.62015	0.83712	0.8558
65	100.93008	0.78436	0.8004
65	203.16221	0.7322	0.7633
65	313.19172	0.68036	0.7034
65	418.88935	0.6279	0.6411
65	516.78963	0.56385	0.5872
65	610.35801	0.50011	0.532
65	706.52557	0.41166	0.4609
65	806.15852	0.29882	0.3233
65	822.61963	0.27381	0.2858
65	904.05884	0.1265	0.1101
65	916.18805	0.10118	0.1019
65	945.64476	0.09142	0.0956

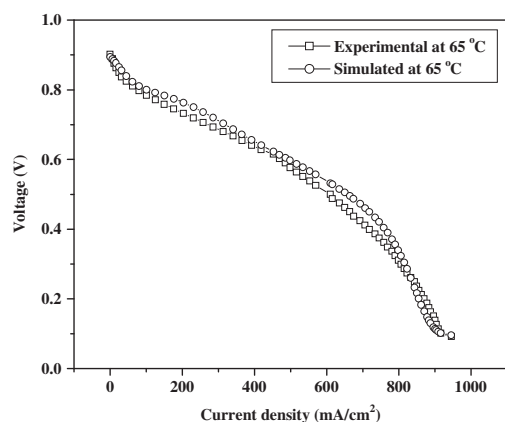


Figure 11. Comparison of polarization curves of experimental and simulated data at 65 °C cell temperature.

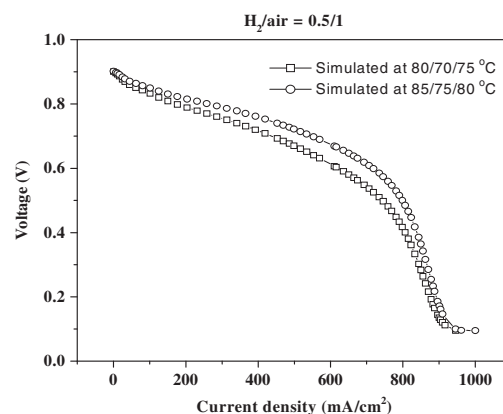


Figure 12. Performance prediction of PEM fuel at 70 and 75 °C cell temperatures.

increase in the mass transfer region. Thus, the aim of the second study is to predict the performance of a fuel cell at higher temperature, which was achieved using ANN and the prediction plots has shown performance improvement in the fuel cell. It is also concluded that there is a significant effect of the number of input parameters on training the network. The more the number of input parameters, the better the network will be trained with less number of neurons; that is, for six input parameters, data network has used four neurons, whereas for four input parameters, data network has used five neurons. So, this work, when compared with the others studies [16], which has used nine neurons with two input parameters, has shown better performance prediction with the less number of neurons. Hence, an ANN simulation method is a helpful tool for predicting the performance of the fuel cell, which is a nonlinear data, at different conditions with less number of experiments. Also, with less number of experiments, the performance of the fuel cell can be estimated at different conditions by using an ANN analysis.

#### 4. CONCLUSIONS

An ANN approach was employed in the simulation of PEM fuel cell and was used to predict the performance of fuel cells. The data for two sets of polarization curves are obtained at different temperatures, and flow rates are used to create and simulate the network. Cell temperature, humidification temperatures, H<sub>2</sub>/air flow rates, and current density were used as inputs, and voltage is used as observed value to train and simulate the network. From the simulated results, it is evident that with the increase of temperature, the performance increases; moreover, with the increase of air flow rate, the performance increases, but at very high flow rates, the performance reduces. Simulated data and experimental data are observed to be in agreement. Also, the number of input parameters has significant effect on training the network. The more the number of inputs, the better the network can be trained with less number of neurons. Further studies are in progress to improve the model.

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