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High power fuel cell simulator based on artificial neural network

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ABSTRACT

Artificial Neural Network (ANN) has become a powerful modeling tool for predicting the performance of complex systems with no well-known variable relationships due to the inherent properties. A commercial Polymeric Electrolyte Membrane fuel cell (PEMFC) stack (5 kW) was modeled successfully using this tool, increasing the number of test into the 7 inputs – 2 outputs-dimensional spaces in the shortest time, acquiring only a small amount of experimental data. Some parameters could not be measured easily on the real system in experimental tests; however, by receiving the data from PEMFC, the ANN could be trained to learn the internal relationships that govern this system, and predict its behavior without any physical equations. Confident accuracy was achieved in this work making possible to import this tool to complex systems and applications.

1. Introduction

A fuel cell is an electrochemical device which converts chemical energy into electrical and thermal energy; Polymer Electrolyte Membrane Fuel Cell (PEMFC) has become popular as power source due of its environmental friendliness and high efficiency. Several models have been proposed to simulate this kind of fuel cell systems based in physicochemical phenomena. Analytical models are an adequate tool to understand the effect of basic variables on fuel cell performance. Many simplifying assumptions are made concerning variable profiles within the cell to develop an approximate analytical voltage versus current density correlation. Semi-empirical models allow designers and engineers to predict the fuel cell performance as a function of different operating conditions (such as pressure, temperature or fuel concentration) using simple empirical equations. Mechanistic models are transport models using differential and algebraic equations whose derivation is based in the electrochemistry and physics governing the phenomena taking place in the cell [1,2]. These models demand high level of knowledge of the process parameters and even though many assumptions must be made in order to simplify them, unfortunately several of these models are not accurate enough. Nevertheless it is

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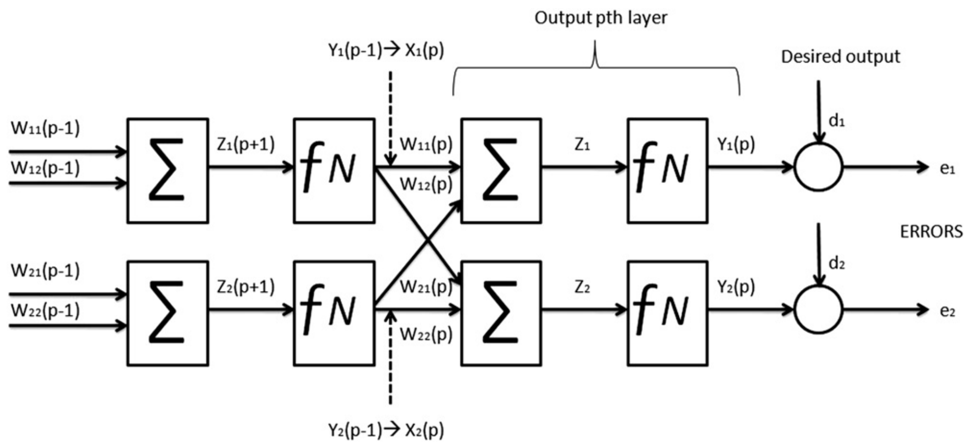

Fig. 1 – A multi-layer perceptron artificial neural network.

possible to achieve performance modeling using black-box models. These models are based on a set of measurable input parameters as current, mass flows, temperature and water flow and they predict the behavior of interesting output parameters such as voltage, and water out temperature. This paper describes the development of an alternative modeling proposal for PEMFC system based on Artificial Neural Network (ANN). Few works of this kind have been reported, Arrigada et al. [3] applied ANN as a modeling tool for evaluation of solid oxide fuel cell performance; Wong-Yong Lee et al. [4] trained ANN models to fit experimental data obtained in a 300 cm^2 single cell in H_2/air operation using Nafion 115 and Nafion 1135 membrane electrolytes. The models take into account not only the current density but also the process variations, such as the gas pressure, temperature, humidity, and utilization to cover operating processes which are important factors in determining the real performance of fuel cells. Jemei et al. [5] proposed a model of PEMFC system of 500 W under 12 V using four inputs (stack current, stack temperature, H_2 and O_2 mass flows) and stack voltage as output. El-Sharkh et al. [6] design a control neural network based on active and reactive power output from a fuel cell power plant; previous work of Shaoduan Ou et al. [7] utilizes a hybrid model (physical and ANN based) for voltage prediction in Direct Methanol Fuel Cell system; Ogaji et al. [8] made an evaluation of ANN based modeling of SOFC taken pressure, current density, fuel and oxidant stoichiometry and anode and cathode temperatures as inputs and voltage, power, temperature and efficiency as outputs; Xiao-Juan Wu et al. [9] developed a non-linear offline solid oxide fuel cell model based in radial basis function neural network; and recently Saengrung et al. [10] investigated the performance prediction of commercial PEM fuel cell (1.2 kW), comparing the use of Radial Basis Function (RBF) and Backpropagation (BP) neural networks. Hatti et al. [12] designed a dynamic neural controller model based with the Quasi-Newton–Levemberg–Marquardt control algorithm based in the manipulation of hydrogen flow in order to reach de active power demand. Bao et al. [9] developed a model to obtain the desired transient performance of air stoichiometric ratio, cathode inlet

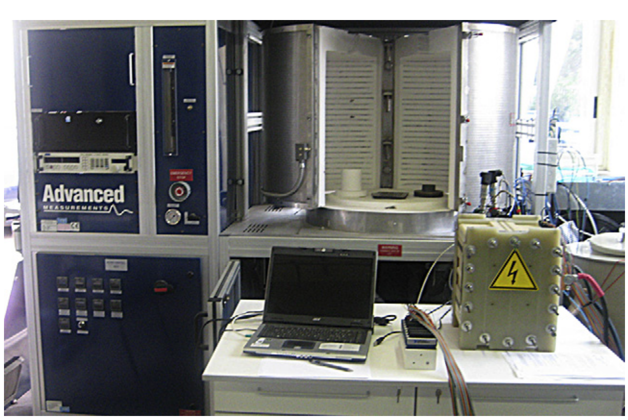

Fig. 2 – NUVERA 5 kW PEM stack, test station and control–acquisition module.

Table 1 – Current stack, and gas flows combinations for the ANN learning set.

CURRENT	STOICH.	10 A	30 A	60 A	90 A	110 A
H_2 flow	1.0	5.00	14.00	28.00	42.00	52.00
N_2 flow	1.0	1.85	5.18	10.37	15.55	19.26
Air flow	1.0	8.30	25.00	50.00	75.00	92.00
H_2 flow	1.2	6.00	16.80	33.60	50.40	62.40
N_2 flow	1.2	2.22	6.22	12.44	18.66	23.11
Air flow	1.2	9.96	30.00	60.00	90.00	110.40
H_2 flow	1.4	7.00	19.60	39.20	58.80	72.80
N_2 flow	1.4	2.59	7.26	14.52	21.77	26.96
Air flow	1.4	11.62	35.00	70.00	105.00	128.80
H_2 flow	1.6	8.00	22.40	44.80	67.20	83.20
N_2 flow	1.6	2.96	8.29	16.59	24.88	30.81
Air flow	1.6	13.28	40.00	80.00	120.00	147.20
H_2 flow	1.8	9.00	25.20	50.40	75.60	93.60
N_2 flow	1.8	3.33	9.33	18.66	28.00	34.66
Air flow	1.8	14.94	45.00	90.00	135.00	165.60
H_2 flow	2.0	10.00	28.00	56.00	84.00	104.00
N_2 flow	2.0	3.70	10.37	20.74	31.11	38.52
Air flow	2.0	16.60	50.00	100.00	150.00	184.00

Table 2 – Input and output variables and ranges after discrimination and separation accordance.

	Input variables	Ranges	Output variables	Ranges
1	I Stack/electronic load	[8.37, 109.94] A	Stack voltage	[33.58, 44.00] V
2	Air mass flow	[10.52, 100.72] slpm	Temp cathode out	[34.39, 74.03]°C
3	Hydrogen mass flow	[4.86, 60] slpm		
4	Nitrogen mass flow	[−0.87, 40.05] slpm		
5	Cathode water injection	[0.1, 12.37] L/min		
6	Temp anode in	[29.63, 57.77] °C		
7	Temp H_2O bulk	[40.14, 58.88] °C		

pressure, and pressure difference between the anode and the cathode based on linearization of the nonlinear dynamic model by linear quadratic Gaussian (LQG) algorithm for set-point tracking, and a model-predictive controller (MPC) with an on-line neural network identifier is also designed to improve robustness.

This work uses state-of-art ANN-based modeling for a more powerful commercial PEMFC (5 kW) system NUVERA Power Flow ™. Because of the high power demands, temperature management was an important issue, so that a Cathode Water Injection (CWI) system (which had not yet been considered in previous studies) was integrated to the model that was also scaled to a more complete set of input variables and two outputs described below, which was expected to achieve a high level of accuracy.

2. PEM fuel cell system

Because of its design and operation mode the PEM fuel cell system has become a main alternative energy source. It consist in a solid polymeric membrane which acts as electrolyte and two platinum porous catalyst electrodes coupled on both sides of the membrane. Cell assembly could be mechanical or pneumatically.

The device in this study was a NUVERA Power Flow ™ 5 kW PEM fuel cell stack consisting of 50 cells each with 500 cm^2 of geometric area, this system works with a CWI system that dissipated heat and humidified the cathode side by mixing air stream and water steam [13]. The the stack was installed with the following main features: appropriate flow rate (air 150 slpm, H_2 55 slpm, N_2 20 slpm), pressure (1 atm) and temperature oxidant and fuel control feeding (preheating anode value 75 °C); appropriate water flow rate (~9 L/min), pressure and temperature (~70 °C) control CWI feed; and an electronic load and cell voltage monitor system (>0.6 V). The system was able to communicate with the user trough a graphic LabVIEW interface built for the control and monitoring program developed by ITAE personnel.

3. Artificial neural networks

Modern non-linear modeling methods as Artificial Neural Networks have been used in many engineering applications such as control systems, pattern recognition and modeling complex process transformations. Input and output data have to be supplied to the network so that it can be trained by using an algorithm that can adjust its internal weights and biases. That multilayer networks are universal tools capable of approximating any measurable function to any desired degree of accuracy. This paper specifies the data acquisition process and ANN's design for a simulation module of a 5 kW PEMFC stack.

An ANN is inspired on the biological model; it can be regarded as a black box able to give certain output data as

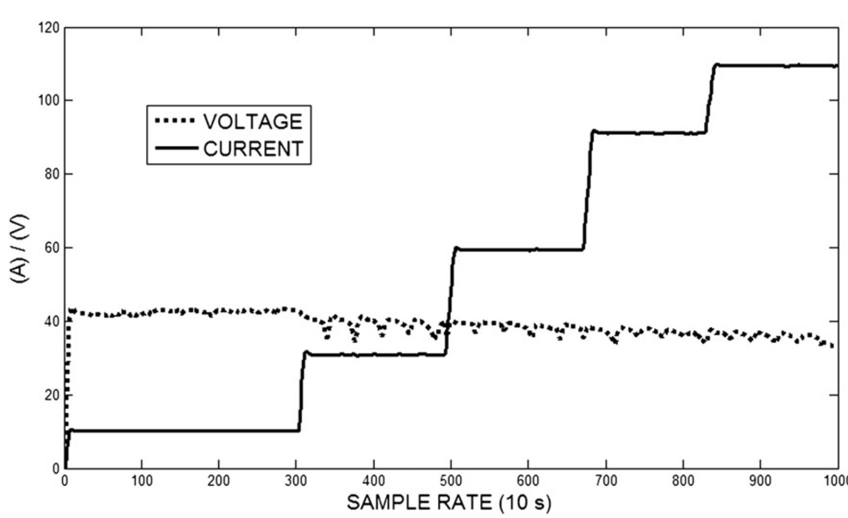

Fig. 3 – Stack current settled by the test station and stack voltage monitored by the monitoring and control system.

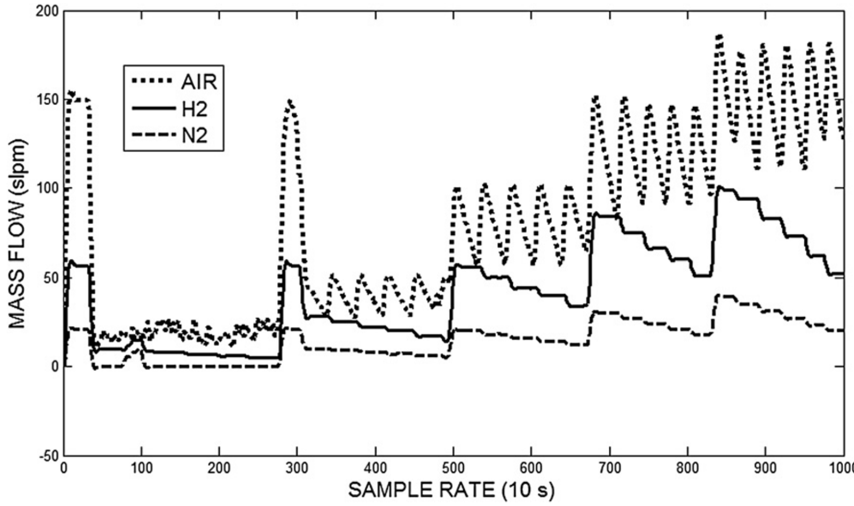

Fig. 4 – Mass flows (H_2, N_2 and Air) controlled and monitored by the test station.

a response to a specific input values combination. Neural networks are widely accepted as a technology offering an alternative way of handling complex problems. They can learn from examples, are fault tolerant in that they are able to handle noisy and incomplete data, as well are able to deal with non-linear problems, and, once trained, can perform predictions at very high speed. The learning algorithm used was Backpropagation (BP) for a multilayer Perceptron network [14]. The BP algorithm starts, necessarily with computing the output layer, which is the only one where desired outputs are available, but the outputs of the intermediate layers are unavailable.

The topology of the network is defined by the organization of the neurons. The multilayer Perceptron network is organized by setting the number of neurons in the input and output layer according to the specific application, and optionally added hidden layers (no theory to determine the amount of layers and neurons for the correct modeling process exists yet) Fig. 1 shows an example of the topology of an ANN.

3.1. *ANN's learning process*

Let η denote the error at the output layer, where:

$$e \triangleq \frac{1}{2}\sum_{k}(d_k - Y_k)^2 \tag{1}$$

$k = 1,2,\ldots,N$, being N the number of neurons in the output layer, d represents the desired output, Y the ANN's output consequently a gradient of e is considered in weights adjustment where

$$\Delta w_{kj}(m) = -\eta \frac{\partial e}{\partial w_{kj}} \tag{2}$$

$$w_{kj}(m+1) = w_{kj}(m) + \Delta w_{kj}(m) \tag{3}$$

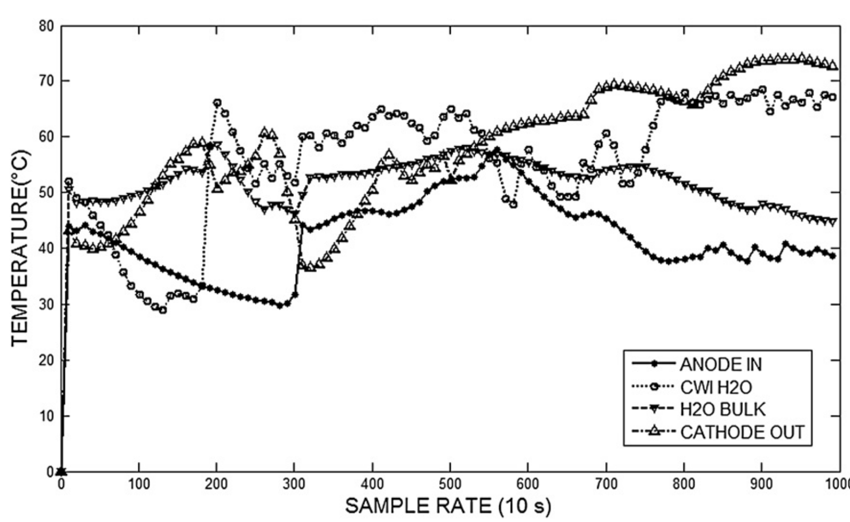

Fig. 5 – Temperature behavior monitored by the control system after preheating values settled on test station.

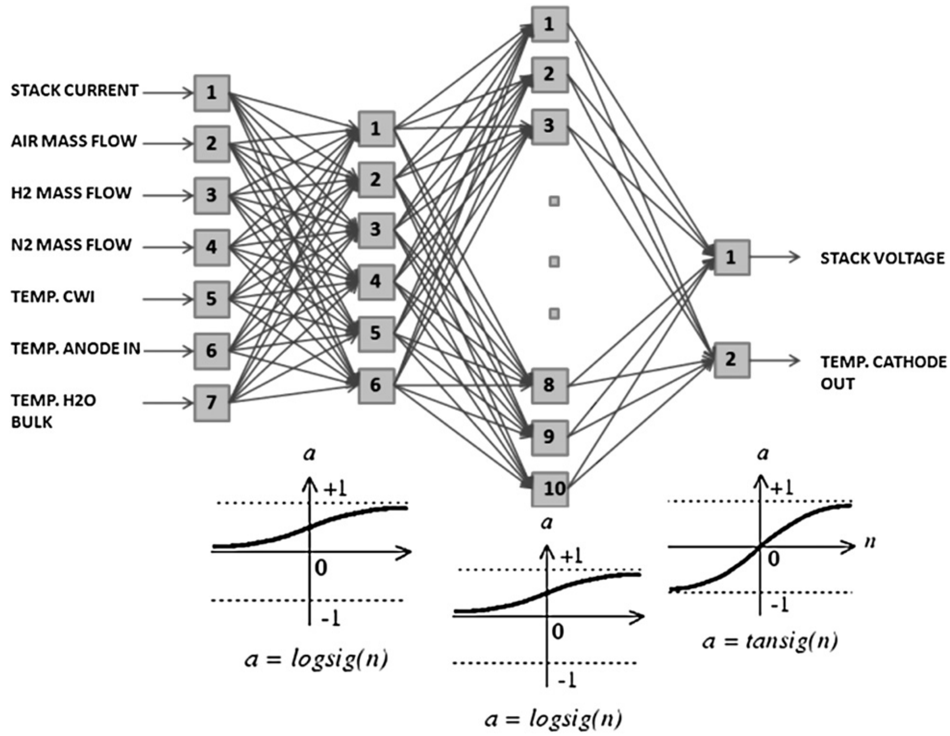

Fig. 6 – ANN's optimized architecture. 7 input variables, two hidden layers with the same logistic sigmoid transfer functions and output layer with tangential sigmoid function.

The learning rate η makes possible to adjust speed and accuracy and the minus ($-$) sign indicates a downhill direction towards a minimum, from the Perceptron definition each neuron receives the numerical information from the input nodes, internally processes it, and gives out an output, the processing is done in two stages, each unit input is weighted and added, and the output is:

$$z_k = \sum_k w_{kj} x_j \tag{4}$$

the result is used as the argument of a linear or non-linear activation function f_N, for the model proposed in this paper logistic sigmoid activation function were used for hidden layers, and tangential sigmoid function for the output layer. This choice results from various test carried out with different activation functions on each layer pursuing and error goal of 0.001.

$$y_k = f_N(z_k) \tag{5}$$

Back-propagating to the *rth* hidden layer, we still have, as before:

$$\Delta w_{ji}(m) = -\eta \frac{\partial \varepsilon}{\partial w_{ji}} y_i(r-1) \tag{6}$$

$$\frac{\partial \varepsilon}{\partial w_{ji}} = -\eta \left[\frac{\partial \varepsilon}{\partial y_{j(r)}} \frac{\partial y_j}{\partial z_j} \right] y_i(r-1) \tag{7}$$

$$\frac{\partial \varepsilon}{\partial y_{j(r)}} = \sum_k \frac{\partial \varepsilon}{\partial z_k(r+1)} \left[\frac{\partial}{\partial y_j(r)} \sum_m w_{k_m}(r+1) y_m(r) \right] \tag{8}$$

where the addition over k is performed over the neurons of the next (the $r+1$) layer that connect to Y_j *(r)*, whereas addition over m is over all inputs to each *k'th* neuron of the $(r+1)$ layer. Initialization of $w_{ji}(0)$ is accomplished by setting each weight to a low random value selected from a pool of random numbers. To accelerate the convergence in learning process, the Levenverg–Marquardt algorithm is used; however special care must be taken to avoid the overfitting phenomena.

4. Modeling PEMFC system by ANN

4.1. *Data acquisition process*

Modeling is usually done with complex models based on the knowledge of physicochemical phenomena. These models only depends on the current, temperature, partial pressures and gas stoichiometries to determine the stack voltage, some parameters such as the water management are not taken into account. Due this limitation, black-box models such as ANNs are adopted in order to consider real measured parameters for a powerful modeling system. Before design the network, one must choose the appropriate network inputs, in order to achieve this, one must understand the process and how each variable affects the performance of the PEMFC outputs, this task is usually done by electrochemical experts. Once the fewest dominant variables are recognized the training process could start, nevertheless is important that training patterns are well distributed

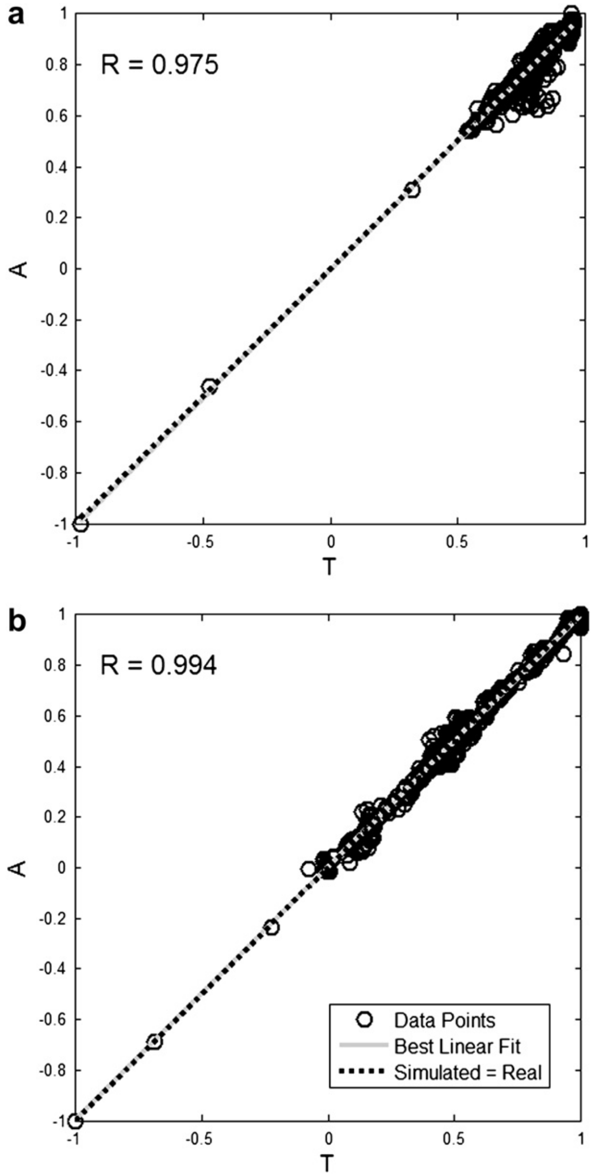

Fig. 7 – Rates of correlation of every output variable (a) voltage and (b) temperature cathode out by linear regression for training.

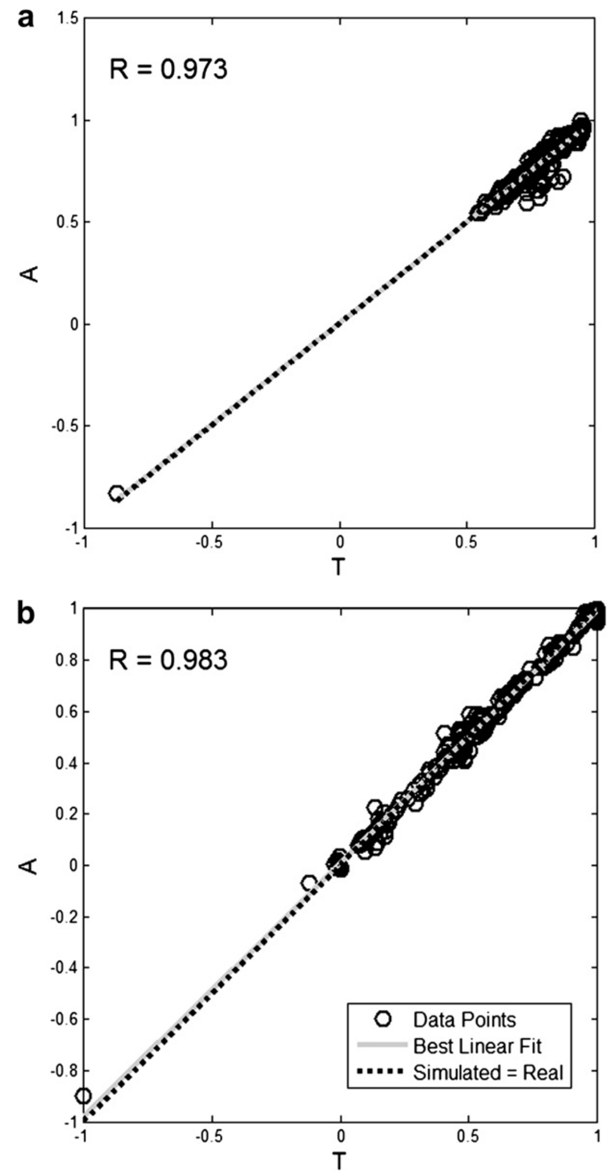

Fig. 8 – Rates of correlation of every output variable (a) voltage and (b) temperature cathode out by linear regression for testing.

throughout the operation range and exposed to a normalization process in order to accelerate the performance prediction.

From the test station and monitor module (see fig. 2), data were obtained from the stack. Due to the high number of operating variables, a complete experimental database of PEMFC system under different operating conditions is difficult to obtain, no model has been able to accomplish yet. In our model three main parameters were varied: H_2 and N_2 gas mixture stoichiometry, air stoichiometry and stack current (Table 1), however more acting variables were observed in order to cover a seven well distributed input space (see Table 2). A monitoring and control LabVIEW™ based system designed under NUVERA considerations was developed for acquisition and control of mass flows, stack voltage, current, pressure and temperature, besides cooling parameters as water temperature and flow initialization settings, This LabVIEW™ based system is capable to monitor every cell tension, temperatures in cathode and anode Inputs and outputs, and to control the pump used for water injection flow.

The test station is used for the experimental validation of the neural model and considers electronic loads, mass flow and pressure sensors and actuators, control and monitor software, besides preheating modules for PEMFC's anode and cathode and AC/DC controllers. Experimental database was obtained setting the anode preheating values on the test station in the range of 75–80 °C.

Table 3 – Best linear fit for training, testing and validation processes.

Process	Voltage best linear fit	Temp. cathode out best linear fit
Training	R = 1.0041 T + 0.0000	R = 1.0227 T − 0.0204
Testing	R = 0.9871 T + 0.0210	R = 0.9791 T + 0.0188
Validation	R = 1.0149 T − 0.0150	R = 1.0677 T − 0.0595

The data structure was fine-tuned for the best running process of the ANN simulator system and it is described below in Table 2. The ANN model is integrated with 7 input neurons for evaluating the stack voltage and cathode temperature (outputs) considering a set of different operating conditions. A simple discrimination process was done on the basis of several test carried. Once this point is considered a pass band filter (low frequency cut of 0.05 Hz to high frequency cut to 1 Hz) was applied in order to attenuate the effects of quick changes in stoichiometry to reestablish the stack when voltage of any of the fifty cells dropped under 0.5 V. The next step was the database division in training data, testing data and validation data, from a total of 1000 accurate measures, half were used to train the network, and the remainder divided in the same amount for testing and validation however this last set was doped with noisy values in the range of [0.85, 1.07] equivalent to 22% of input values variation in order to size the robustness of the model [6]. The input and output variables for the ANN's learning and function were normalized to be within a [−1, 1], this process was necessary for the better convergence of the neural model however minimum and maximum values of the training data were used for testing and validating data.

Figs. 3–5 show behavior of every variable during the acquisition time before being separated to input and output variables.

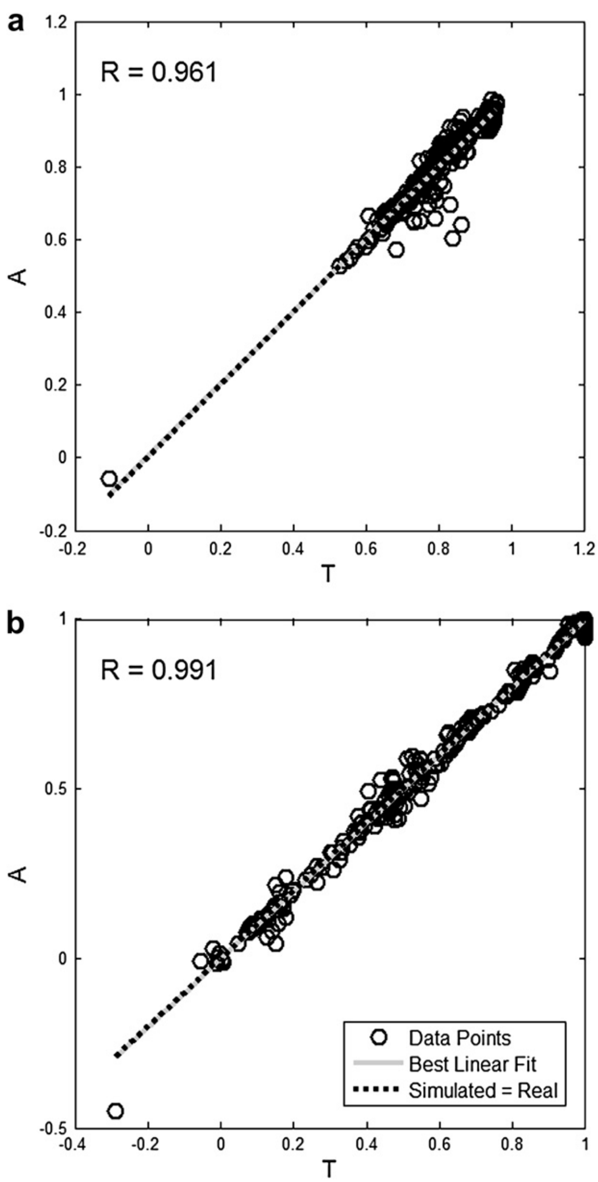

Fig. 9 – Correlation rates for validation patterns of every output variable (a) voltage and (b) temperature cathode out.

5. Results and discussion

As mentioned before the ANN training was realized trying several architectures, training algorithms and transfer functions, in order to reach the error goal = 0.001, the 7-6-10-2 architecture (Fig. 6) brings fast and very accurate approach to the intelligent simulation system. Both hidden layers use logistic sigmoid transfer function, the output layer gives the simulated values using tangential sigmoid transfer function. ANN's backpropagation Levenverg Marquardt algorithm has been proved experimentally and is the more suitable method according to literature [10,11,14].

After comparing several architectures, the ANN learned considerably fast to reach the error goal, linear regression of every output and every set (training, testing and validation) was calculated in order to observe correlation between experimental data and simulated data from the ANN model. Observing in the training session, a minimum correlation rate of $R = 0.975$ (Fig. 7a) was gotten from the voltage variable, the other output (Cathode temperature out) presents better correlation (Fig. 7b), indicating the success of training, in order to verify that the adequate training is necessary to propagate some testing patterns, this process shows an excellent behavior as it seen in Fig. 8, again minimum correlation rate was reached for the voltage variable $R = 0.973$ (fig. 8a). These results make us to trust in the best ANN performance to simulate, however it is necessary to test them by using another set of experimental data doped with a noise matrix in the range described above. In addition to correlation rate, the best fitting lines obtained for the three processes are described in Table 3.

A sequence of incremental current steps from 10 to 110 A and several stoichiometry gas combinations were propagated trough the neural model in order to observe and compare the simulated results against experimental data. Excellent modeling performance of the neural network simulator can be observed in Fig. 9 where validation patterns doped with noisy data have shown excellent fitness to real data; again the first

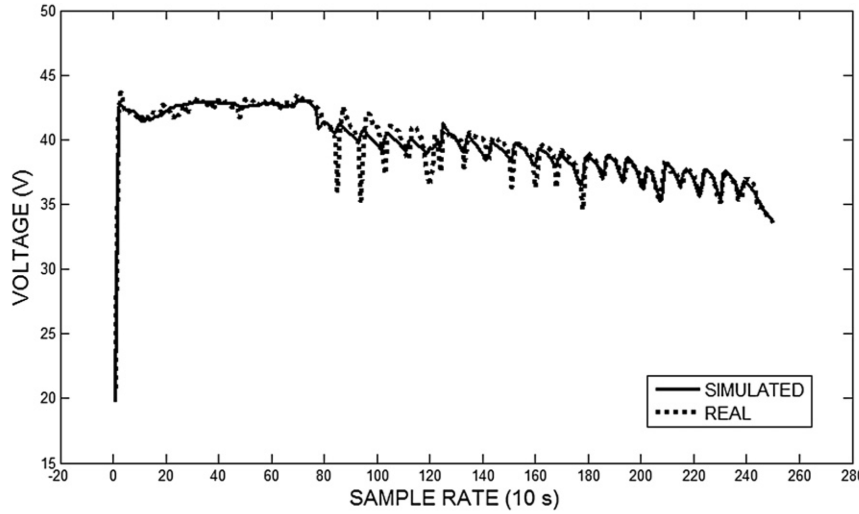

Fig. 10 – Stack voltage behavior comparison between real and simulated sequences.

variable (Fig. 9a) shows the minimum rate value of 0.961 (0.014 below training correlation), the second variable (Fig. 9b) presents again acceptable performance in this process, however in order to illustrate the prediction accuracy of the modeling tool, Figs. 10 and 11 represent the sequence of real and simulated output data voltage and temperature when the mentioned input sequence is propagated through the network.

As steps in the current increase, voltage drops gradually. In the experimental range, however, even though variations up to 22% were induced into the neural model, the tendency follows the same that real data which establish the robustness of the network. The same phenomena occurs in the temperature output, which again as long as the power demand increases its slope increase, this oscillating naturalness is caused by the compensating effect of the CWI system. However, again, the neural model follows in a narrow way the behavior of experimental sequence and in order to set numerically this performance, it is necessary to calculate the simulation error.

The error associated to each distribution was calculated by the Mean Square Error (MSE).

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(A - T)^2 \tag{9}$$

where A represents the simulated data vector for every output parameter and T the real experimental values taken from the stack. For every output value in the validation set, the errors obtained from comparing real values versus simulated data were: Stack Voltage = 0.9815 V (9.4%), Cathode Out Temperature = 2.2177 °C (5.6%).

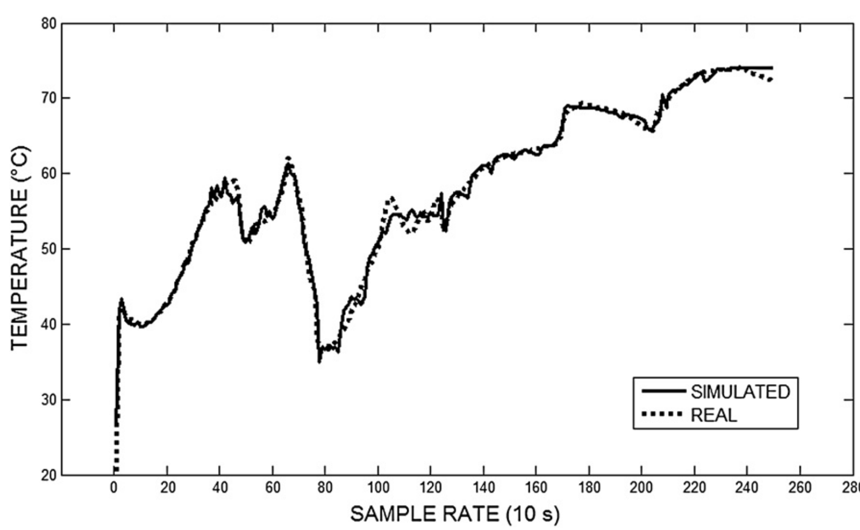

Fig. 11 – Cathode out temperature between real and simulated sequences.

6. Conclusions

Modeling is an important tool dedicated to the study of the systems and observation of them under several applications in order to optimize their performance saving time and resources. When modeling is done by using experimental data which cover $N \times M$ dimensional space, excellent performance prediction could be achieved by artificial neural networks due to their capabilities of learning, adapting and tolerating a lack of information. Modeling of a NUVERA 5 kW stack was developed using ANNs as alternative approach to model a fuel cell system when physical variables relationship is not well known. The Artificial neural network designed in this work shows excellent accuracy in modeling and prediction for this particular 5 kW performance, considering a 7 input 2 output dimensional space the maximum error gotten from every output parameter was a 9.4% in the stack voltage prediction and a 5.6% from the Cathode Temperature Out. Confidence and robustness were achieved by introducing noise to experimental data. Previous papers based on similar techniques do not consider such amount of parameters, they also promote scaling of this kind of modeling techniques to high power systems, however this scaling is not simply. This study illustrate the temperature behavior of high power PEMFC and the interaction of a CWI system. Such work will be more helpful to model more complex systems and PEMFC applications simply by introducing this black box FC model.

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