고분자 전해질 연료전지의 운전특성 예측을 위한 reduced order model

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Development of Reduced Order Models (ROM) for Timely Prediction of the Behavior of Proton Exchange Membrane Fuel Cells

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1. Introduction

Proton exchange membrane fuel cells (PEMFC) are considered one of the most promising sources of distributed electrical power. Detailed modeling of PEMFC has been of considerable interest in predicting the performance of these fuel cells and use in various systems engineering activities. Computational Fluid Dynamics (CFD) models have the promise of providing detailed information about the operation of fuel cells and have been used in fuel cell modeling [1]. While CFD equipment models provide detailed analysis of the performance, they are very time-consuming to develop and run. The computations become quite complex when such models have to be embedded in flowsheet level optimization. Hence, there has been recent interest in building Reduced Order Models (ROMs), based on detailed CFD simulations, that can be routinely used in a number of performance studies [2].

In this paper, we will present results on building reduced order NN models for predicting the flow of reactants in a proton exchange membrane fuel cell manifold. A feed-forward, back-propagation neural network is used in this work. The data for NN training is generated from detailed CFD simulations of the manifold using Fluent. The input parameters to the NN are: channel dimension, inlet velocity, inlet gas temperature and humidity. The ability of the network to quickly predict detailed flow behavior in the manifold will be discussed in this paper.

2. Development of Reduced Order Models

2.1 Architecture of ANNs

The structure of a feed-forward multilayer neural network chosen in this case consists of an input layer, a hidden layer, and an output layer. Each input parameter is indicated by a node in the input layer, and no data processing occurs here, i.e., the input nodes only act as collectors of the input signals ($x_1; \ldots ; x_M$). After that, the information is distributed from every input node to every unit in the hidden layer, and it is amplified or debilitated by the synaptic connections between them, i.e., the weights (w_{ji}). The pieces of information that arrive at the hidden units are summed up by the summation function, P, and transformed by the transfer function,

F. From the hidden layer, the data is re-distributed and weighted by a new set of weights (w_{kj}), and then passed on to the processing units in the output layer, where the information is summed up and transformed once again, generating the output signals (y_1; . . . ; y_N). An extra input equal to unity is fed both to the hidden and the output layers, and its corresponding weight introduces an off-set or bias to the transfer function. The ANN shown in Fig. 1 is a two-layer network, since only two layers have processing units or artificial neurons. Eventually, every output can be represented by a generic expression of the inputs, e.g., for a network with M input signals, H neurons in the hidden layer and N outputs [2,3]:

$$y_k = F_0\left(\sum_{j=0}^{H} w_{kj} F_h\left(\sum_{i=0}^{M} w_{ij} x_i\right)\right) \qquad \text{where } k=1,\ldots\ldots,N \qquad (1)$$

The weights are fixed by minimizing a mean square error (MSE) objective function, E, given by:

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(e_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(t_i - a_i)^2 \qquad (2)$$

where t is a target value and a is a network output

During the training procedure, local gradients of E with respect to the weights are calculated to update the weights. The weights, which at the beginning are random numbers close to zero, are successively updated in the direction of the decreasing error gradient till convergence.

$$\Delta w_{ij} = -\eta \frac{\partial \mathrm{E}}{\partial w_{ij}} \qquad (3)$$

$$\Delta w_{ij} = -\eta \frac{\partial \mathrm{E}}{\partial w_{kj}} \qquad (4)$$

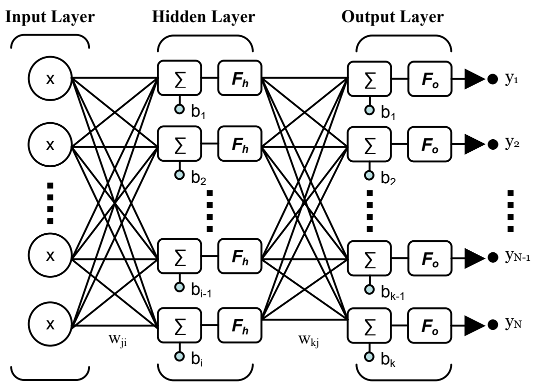

Fig. 1. The feed-forward, multi-layer neural network.

The inputs used in our work are: rib width, gas inlet temperature, initial pressure and fuel flow rate. The outputs used in this study are: H_2 consumption, pressure drop of the manifold and mean velocity of the channel. To optimize the network, the number of hidden neurons, the number of training epochs and the learning rate are altered during the training phase by a trial-and-error method.

2.2 Data set for training

Since we are interested in developing a reduced order model, data for the reduced order model are generated through CFD simulations of a PEMFC in Fluent. This data is used for the training of the ANN-based simulator. The CFD model was used to generate data for approximately 192 different operational cases. The main operational parameters of the cell, such as mass flow rate (0.5–2), inlet gas temperature (60–120 ℃) and initial pressure (2-5 atm), are varied for the data generation. In all the simulations, the inlet gas was assumed to be fully humidified. To consider various configuration of the manifold, wide rages of rib width (0.5-2 mm) were simulated.

2.3 Half cell model

We demonstrate our proposed approach on a half cell model for the anode side of the fuel cell. The domain for the half cell model of PEMFC consists of gas flow channel, gas diffusion electrode and catalyst layer. The manifold configuration was assumed to be serpentine in shape with rectangular cross section channels. The hydrogen gas entering the manifold is fully humidified. For more information on the half cell model, see [4].

3. Results

Fig. 2 shows the proposed ANN-based, reduced order model structure that is used in this work. The neural network was trained with an improved version of the backpropagation algorithm, i.e., the Levenberg–Marquardt algorithm. During the learning process, the error function was minimized with an increasing number of training epochs, as shown in Fig. 3. An epoch is a cycle that is finished when all the available training input patterns have been presented to the network once. Each of the points in the 3D graph is drawn by scatter method: x-direction is H_2 consumption, y-direction is mean velocity of fluid in the manifold and z-direction is pressure drop.

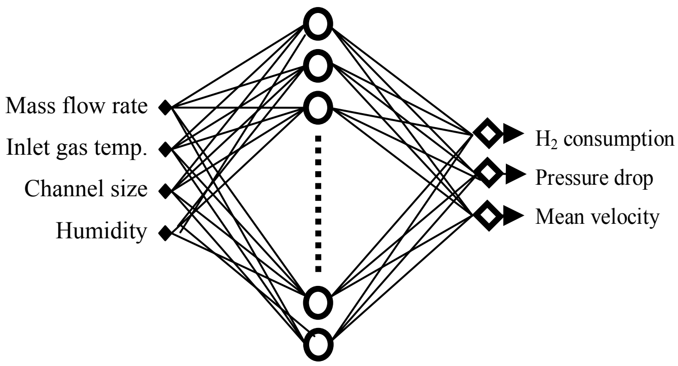

Fig. 2. Proposed neural networks structure.

4. Conclusions

This paper introduces a technique based on neural network to predict the performance of PEMFC. The artificial neural network showed very good predictive capabilities. The ANN model is much faster and easier to use, which makes it suitable for the prediction of the performance of PEMFC than a detailed CFD model.

Such a reduced order model could be used in lieu of the detailed CFD model in a number of systems engineering calculations.

Acknowledgement
This work was supported by Korea Science and Engineering Foundation (R08-2003-000-10982-0) and Korea Research Foundation.

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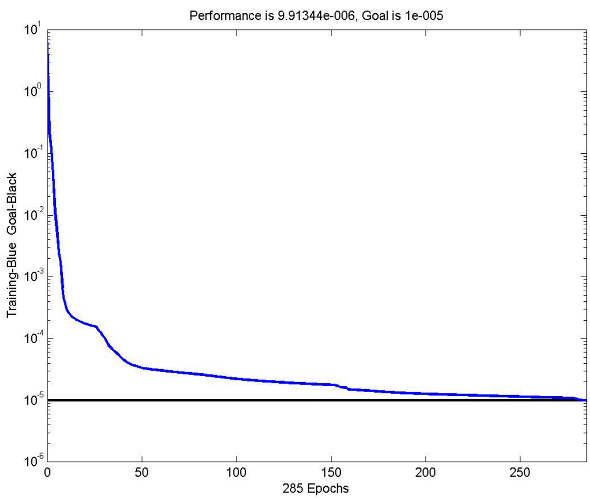

Fig. 3. Training errors during ANN training process.

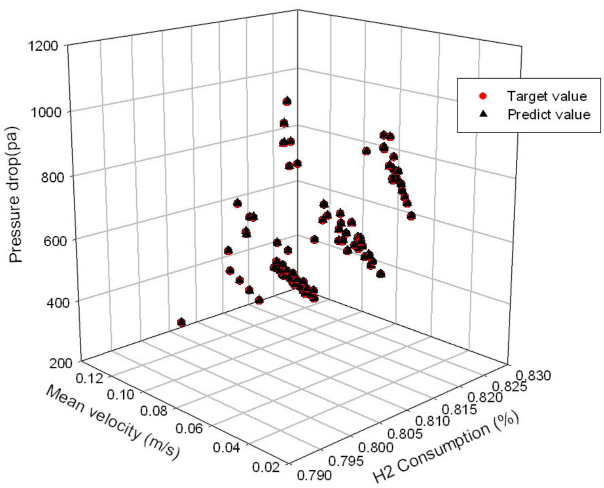

Fig. 4. Comparison of physical models and ANN model.