KIGAS Vol. 10, No. 2, June, 2006
(Journal of the Korean Institute of Gas)

Time-Efficient, Repetitive Predictions of the Performance of PEMFCs Based on a Neural Network-Based, Reduced Order Model

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(Received 15 June 2006, Accepted 23 June 2006)

Abstract: Detailed modeling of PEMFCs has been getting considerable interest for predicting the fuel cell performance and also for use in various systems engineering activities. While CFD-based equipment models provide detailed analyses of the performance, they are very time-consuming to develop and run. The computations become quite complex when such models have to be embedded into the flowsheet-level optimization of fuel cell systems. In this paper, we present results about building and using NN-based reduced order models for quickly and repetitively predicting the flow of reactants in a PEMFC manifold.

Key words: Fuel cell, Reduced order model, Modeling and simulation, Computational fluid dynamics, Performance analysis

I. Introduction

Fuel cells are devices that convert the chemical energy of reactants (hydrogen and oxidant) directly into the electrical energy. They operate like batteries, but they have a high energy conversion with low emissions. In those reasons, they became a prime candidate for powering of the next generations [1,8]. The polymer electrolyte membrane fuel cell (PEMFC) is seen as a system of choice for automotive applications due to several advantages this fuel cell offers over other types. PEMFC operates at low temperatures, allowing faster start-ups and immediate response to changes in the power demand.

The overall performance of PEMFC is determined by many factors, including material properties, manufacturing techniques and the fuel cell design itself [11]. The involving complexities and difficult experimental environment of fuel cell systems have encouraged such simulation-based approaches to develop models that could simulate and predict multi-dimensional coupled transport of reactants, heat, and charged species using Computational Fluid Dynamic (CFD) methods [3,4,13].

Building equipment models based on CFD studies is starting to become widely accepted. While CFD equipment models could provide detailed analysis of the performance, they are very time consuming to develop and run. The computations become even more complex and requiring bigger computational resources when such models have to be embedded into flowsheet-level optimizations. Hence, there has been recent interest in developing Reduced Order Models (ROM), based on detailed CFD simulations, which would be more easily and time-efficiently used in numerous performance studies.

In this research, we investigate on developing reduced order models for repetitive and time-efficient simulations of the performance of fuel cells and applying them to the integrated design, optimization, operation and control of fuel cell systems. We will present results on building Artificial Neural Network (ANN)-based reduced-order models for predicting the flow of reactants in a proton exchange membrane fuel cell manifold. A feed-forward, back-propagation neural network is selected and used in this work. The data for ANN training are generated from the detailed CFD simulations of the manifold using a half-cell model, which is also developed as part of this research. The ability of the developed ROM to predict the detailed flow behavior in the manifold will be discussed as a validation of the proposed approach.

II. CFD-based Fuel Cell Modeling and Simulation

2.1. Half Cell Modeling of PEMFC

Since such a situation is assumed that sufficient experimental data on operating fuel cells are not available or hardly obtainable, a physical half cell

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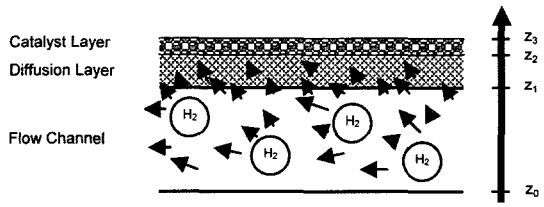

Fig. 1. Schematic of a half cell model of PEMFC.

model of PEMFC is used to generate the data required for the training of the ANN [2]. The problem domain for the half-cell model of PEMFC consists of three different zones: (1) flow-field channels (serpentine design) which are imprinted onto the bipolar plates; (2) gas diffusion electrode; and (3) catalyst layer.

Fig. 1 shows the half cell model presented here. It is assumed that fuel is hydrogen on the anode side. The hydrogen gas enters the domain at gas inlet in the bipolar plate. The flow-field in the bipolar plate helps the distribution of hydrogen reactant gas onto the surface of the electrode. The gas is transported towards the anode electrode via diffusion and convective transfer. The next layer is the catalyst layer, where hydrogen molecules break into the protons and the electrons. It was decided to choose the rectangular cross-section channels for studying the effect of channel dimensions. The flow-field was chosen to be single-path serpentine design.

2.1.1. Model Assumptions

The complete fuel cell model is an extremely complex system. In order to devise a numerically-tractable, three-dimensional half cell model presented here, it is necessary to invoke a number of simplifying assumptions. The followings are the assumptions made in this study:

(1) Steady state and stationary conditions exist in the single cell stack. The effect of gravity is also neglected.

(2) Isothermal conditions exist in the cell domain.

(3) Based on the Reynolds number calculation, the flow in the fuel cell is laminar. Hence, all the transport equations are formulated for laminar behavior.

(4) The permeability of the electrode material is assumed to be isotropic and has a value of 10^{-12} m^2.

(5) The volume of the by-product liquid H_2O is assumed to be negligible in the domain.

(6) Since the density of the reactant gas (H_2) varies from location to location in the domain, compressible gas technique (in Fluent) is used to determine the density of the gas mixture.

2.1.2. Governing Equations

The basic transport equations (conservation of mass and momentum) were written for each of the zones of the domain. The conservation of mass, also called equation of continuity is given by:

$$\frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z) = S_m \tag{1}$$

where ρ is the density of the fluid in the medium and v_x, v_y and v_z are the components of the velocity in x-, y-, and z-direction, respectively.

The source term, S_m appears due to the electro-chemical reaction and corresponds to the consumption of hydrogen, and is given by [9]:

$$S_m = 0 \qquad Z_0 \le Z \le Z_2 \tag{2}$$

$$S_m = \frac{\lambda C_{H_2}}{k + C_{H_2}} \qquad Z_2 \le Z \le Z_3 \tag{3}$$

where $[C_{H2}]$ denotes the concentration of hydrogen in the domain, λ and k are terms that have no physical meaning and their values depend upon the rate constants for the atomic oxidation of H_2 and platinum loading in the catalyst layer. As discussed in [7,9,15], the value of k was set equal to 1. Since the value of λ may change from one fuel cell system to another, we will present cases corresponding to different values of ρ. It was decided to choose the value of λ as 20 for the simulations discussed in this paper.

The conservation of momentum, also called as Navier-Stokes equation, is given by:

- momentum (x-direction)

$$\rho\left(v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) = \\ = -\frac{\partial P}{\partial x} + \mu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right) + S_{px} \tag{4}$$

- momentum (y-direction)

$$\rho\left(v_x\frac{\partial v_y}{\partial x} + v_y\frac{\partial v_y}{\partial y} + v_z\frac{\partial v_y}{\partial z}\right) = \\ = -\frac{\partial P}{\partial y} + \mu\left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2}\right) + S_{py} \tag{5}$$

- momentum (z-direction)

$$\rho\left(v_x\frac{\partial v_z}{\partial x} + v_y\frac{\partial v_z}{\partial y} + v_z\frac{\partial v_z}{\partial z}\right) = \\ = -\frac{\partial P}{\partial z} + \mu\left(\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2}\right) + S_{pz} \tag{6}$$

The source terms in the above equations arise due to the pressure difference when the fluid passes through a porous medium. So these terms exist only for electrode and catalyst zones in the domain. The source term, for low velocities of fluid, typical to those in fuel cells, is given by Darcy's law:

$$S_{px} = -\frac{\mu}{\alpha_x} v_x, \quad Z_1 \le Z \le Z_3 \tag{7}$$

$$S_{py} = -\frac{\mu}{\alpha_y} v_y, \quad Z_1 \le Z \le Z_3 \tag{8}$$

$$S_{pz} = -\frac{\mu}{\alpha_z} v_z, \quad Z_1 \le Z \le Z_3 \tag{9}$$

where μ is the viscosity of the fluid in the medium, and α is the permeability of the electrode material. Since the permeability of the medium was assumed to be isotropic, each of α_x, α_y and α_z has a value of 10^{-12} m^2.

2.2. Generations of the Cases from CFD Simulations

Since such a situation is assumed that sufficient experimental data on operating fuel cells are not available or hardly obtainable, the developed half cell model of PEMFC is used to generate the data required for the design and training of the ANN-based ROM. The model was run to simulate approximately different 192 operational cases. Main operational parameters of the cell and their changed ranges are (1) rib size of the flow field (0.5, 1.0, 1.5, 2.0 mm), shown in Fig. 2, (2) inlet gas temperature (60, 80, 100, 120°C) and (3) gas flows, while inlet gas was maintained as fully humidified flow. The mass flow rate (0.5, 1.0, 1.5, 2.0 kg/s) is varied in each case in order to obtain the required fuel utilization. The initial pressure (2, 3, 5 atm) is also varied for each case.

The model equations were solved using a commercial CFD software, Fluent 6.1, with Gambit as preprocessor. Control volume technique was used for solving the problem. The domain was divided into hexahedral volume elements. The total number of volume elements in the flow-field distributor depends on the rib size and varies from case to case. In the gas distribution electrode and catalyst layer, the total numbers of volume elements were 102,400 and 25,600, respectively. A grid adaptation technique was used to obtain a solution, which is independent of the dimensions of the chosen grid.

The source terms were incorporated into Fluent through the introduction of user-defined function (UDF) codes written in C language. The whole solution procedure is as follows: Momentum equations were solved for the velocity. This was followed by solving of equation of continuity, which updates the pressure and flow rate. Results were then checked for convergence. Since the density of the hydrogen gas varies from point to point, a technique similar to ideal gas technique was used for solving the model.

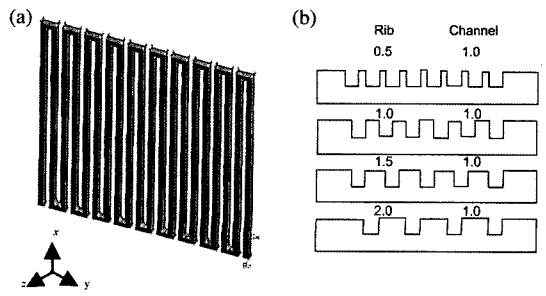

Fig. 2 (a) Serpentine flow-field design, (b) Rib and channel configurations used.

III. Development of Reduced Order Models

3.1. NN-based ROM

Among many possibilities of building reduced order models, ANNs are an attractive choice. ANNs are software systems modeled after the human process of learning and remembering. They mimic the cognitive neurological functions of the human brain: They are capable of predicting new observations from historical samples after executing a process of learning. The advantage of neural networks lies in their inherent ability to deal with various samples of input data and to learn quickly. ANNs have been used in a wide range of engineering applications, such as pattern recognition, human behavior modeling, signal/image processing and function approximation [6,10,12]. There are literally hundreds of neural network architectures, which set the way how internal connections are made and learning processes occur. Backpropagation architecture, introduced

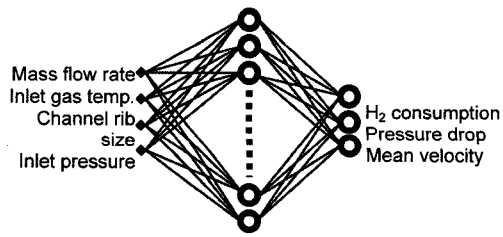

Fig. 3. Structure of the developed ANN-based ROM.

in 1974 and still one of the most dominant forms of all neural networks [10], has been used in this research.

Fig. 3 shows the structure of the ROM developed based on the two-layer, feed-forward NN. Input parameters are mass flow rate, inlet temperature, rib size and initial pressure; output parameters are H_2 consumption, pressure drop and mean velocity.

3.2. Training and Validation

To be able to produce the correct output values, the properly designed structure of a neural network was trained with an improved version of backpropagation algorithm, the Levenberg–Marquardt algorithm, using Matlab Neural Network Toolbox [5,14]. During the learning process, the error function (MSE) was minimized with an increasing number of training epochs, as shown in Fig. 5. An epoch is a cycle that is finished when all the available training input patterns have been presented to the network once. To optimize the performance of the NN, the number of hidden neurons, the number of training epochs and the learning rate were altered during the training phase by a trial and error method.

Once the ANN provided a satisfactory output, validation was carried out with a test set (randomly selected input data, i.e. new operational points with H_2 consumption, initial pressure, mass flow rate and temperature). After this final test, the network was ready to generate predictions of the behavior of the PEMFC for a broad range of conditions. Half of the operational points were used to train the ANN, while the other half was used for the validation.

IV. Results and Discussions

The full-scale, CFD-based physical model was used to get simulation results for approximately 192 different operational cases. Main operational parameters of the cell that were varied are rib size of the flow field, shown in Fig. 2, inlet gas temperature, the mass flow rate, and the initial pressure. The required computation time for a case of simulation is shown in Table 1. Fig. 4 shows one of the simulation results obtained for rib width = 0.5 mm, flow rate = 1e-07 kg/s, inlet pressure = 2 atm, and temperature =333 K.

Pressures are monotonically decreasing following the channel length from inlet to outlet and the magnitudes of the overall pressure drops decrease as the rib width increases. Increasing the rib width results as the decrease in the total length of the channels (or the number of channels), and hence the pressure drop in the channels decreases. When the rib width is 0.5

Table 1. Comparison of computation times required for performance predictions.

Full CFD Simulations				ANN-based ROM
Rip size (mm)	Number of nodes	Number of elements	Mean simulation time (min)	
0.5	239,746	67,360	15	~1 sec.
1.0	221;066	52,416	13	
1.5	208,546	42,400	12	
2.0	202,426	37,504	10	

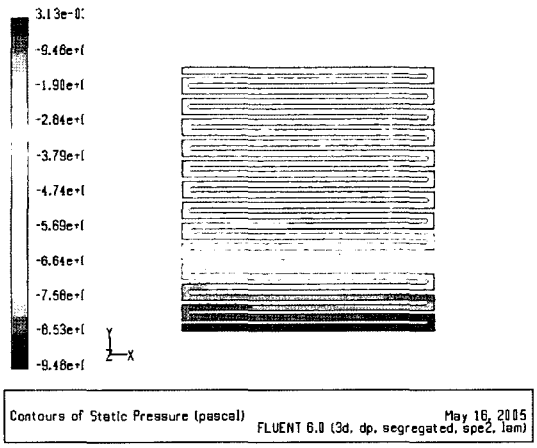

Fig. 4. Pressure distribution in the anode channel for rib width = 0.5 mm.

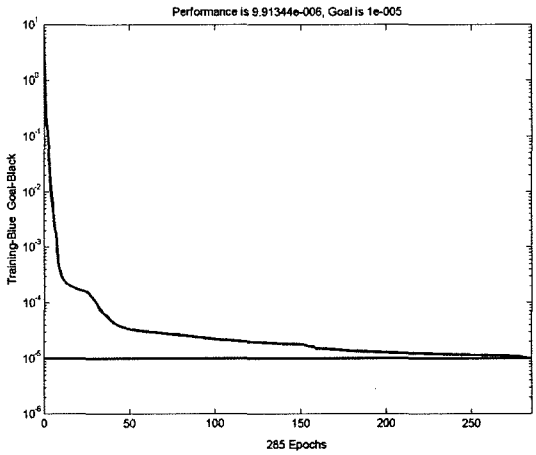

Fig. 5. Change of MSE training error during the learning process.

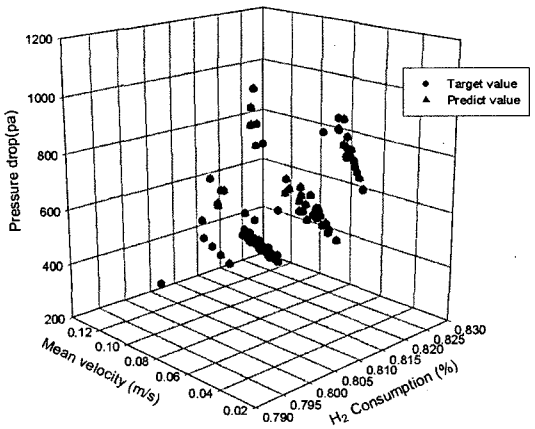

Fig. 6. Comparison of predicted values from ROM and CFD simulations.

mm, the pressure drop is the largest among four cases. The pressure drop is the smallest with the rib width of 2.0 mm.

In Fig. 6, the CFD simulation result points are denoted as circles, while the result generated by the ANN-based ROM is shown as triangle. The concordance between both models is clear: The average discrepancy between the physical CFD model and the ROM are less than 1%.

Even though the ANN model has taken a certain amount of time for training and validation, once it is obtained, it quickly returns the prediction results, as shown in Table 1. One run of a full CFD simulation usually takes over 10 min. Needless to say, the more increase in the number of elements and the node, the more increase in time to generate results. Total computation time required for a performance prediction using the full-scale CFD simulation method increased in accordance with the number of elements, but when the ROM was used, it always took below 1 sec. For the case of rib width = 0.5 mm, the number of elements was the most; the CFD simulation had taken 15 min in this case whereas using the ANN model had taken below 1 sec.

After the analysis of the results so far achieved, it is quite clear that the developed ANN-based ROM is much faster and easier to use when many number of simulation results of fuel cells are to be obtained at various operational conditions. This makes it suitable as a tool for the repetitive and time-efficient generations of performance predictions required for the continuing system-level studies (e.g., design, optimization and control studies) of fuel cells.

V. Conclusions

The ANN-based, reduced-order model of half-cell PEMFC showed a good congruence with the full-scale CFD-based model, which was used by running its simulations to generate the data set for the design, training and validation of the reduced-order model: The average values of the error for trained cases were well below 1%. Besides the sufficient numerical accuracy, the developed ANN model is so much faster (~1000 times fast) and easier to use than the complete CFD simulations that it becomes more suitable for the repetitive, time-efficient uses in performance predictions. Based on the analysis of H_2 consumptions, it was found out that the selected design of the fuel cell shows the best performance when the rib width = 1.0 mm.

The developed ROM also showed good prediction results over wide ranges of operational conditions, which are not fully covered during the training. Once a CFD-based model is built, continuing design and optimization of the fuel cell system can be done in more cost and time-efficient way by using this ROM-based methodology, even before the physical system becomes available for the collection of experimental data. The suggested method of developing and using the ROM, in an integrated way, for the system-level studies is being further automated and developed as a plug-in module of design suites for fuel cells.

Acknowledgements

This work was supported by the Korea Research Foundation Grant funded by the Korean Government (R08-2003-000-10982-0).

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