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New hybrid model of proton exchange membrane fuel cell*

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Abstract: Model and simulation are good tools for design optimization of fuel cell systems. This paper proposes a new hybrid model of proton exchange membrane fuel cell (PEMFC). The hybrid model includes physical component and black-box component. The physical component represents the well-known part of PEMFC, while artificial neural network (ANN) component estimates the poorly known part of PEMFC. The ANN model can compensate the performance of the physical model. This hybrid model is implemented on Matlab/Simulink software. The hybrid model shows better accuracy than that of the physical model and ANN model. Simulation results suggest that the hybrid model can be used as a suitable and accurate model for PEMFC.

Key words: Proton exchange membrane fuel cell (PEMFC), Artificial neural network (ANN), Hybrid model, Physical model
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INTRODUCTION

Fuel cell is an electrochemical device in which fuel and oxidant react in a controlled manner to produce DC electricity, water and heat. The fuel cell, since its appearances, has become a good alternative to conventional internal-combustion engine. Fuel cell had hold promise for reducing some national reliance on a petroleum-based energy policy and government and industry are combining forces to bring fuel cell technologies to the industry. Fuel cell is increasingly being installed to power schools, municipal, commercial buildings and portable power source. Future applications also include field hospitals and buildings in remote locations, computers and appliances, residences and military locales (http://www.engr.uconn.edu/soe.php?pId=ctfcresgeneral).

Fuel cells can be divided into six types according to different type of electrolytes used. Among them, proton exchange membrane fuel cell (PEMFC) is believed by most experts to be the best candidate for many applications due to its high efficiency, high power density, low operating temperature, long life, and ability to tolerate air (Mehta and Cooper, 2003).

Although PEMFC has so many advantages, reducing the cost and enhancing their efficiencies remains a problem. To improve the fuel cell system performance, design optimization and analysis of fuel cell systems are important. Physical model and simulation are good tools for design optimization of fuel cells, stacks, and fuel cell power systems. Recently, physical model and computer simulation were used to gain better understanding and improving fuel cell performance (Costamagna, 2001; Dutta *et al.*, 2000). Physical model is useful for simulating the inner details of PEMFC, but most physical models either require too extensive calculation or are not accurate enough. Besides, physical model may not be available to describe some input-output relations, such as Pt loading, humidity, and other design or operating parameters. It is important to have an adequate model to estimate the overall performance of a PEMFC without the need for extensive calculation.

An appropriate artificial neural network (ANN) model provides useful and reasonably accurate input-output relations. ANN has been extensively em-

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ployed in various areas of science and technology because of its wonderful multi-dimensional mapping capability. ANN based PEMFC model and SOFC model are presented in (Jemeï *et al*., 2003; Ogaji *et al*., 2006). When experimental data are inadequate, it is difficult to obtain well-trained ANN model. So, a hybrid model was addressed by Ou and Achenie (2005). Compared with the previous models, the hybrid model need less time and less training data to achieve the equivalent accuracy.

In this paper, a general description of PEMFC system architecture is presented first and then hybrid model including physical component and ANN component is proposed. Finally, simulation results from the proposed hybrid model are compared with the experimental data, ANN model and physical model.

PEMFC SYSTEM

Principle and configuration of PEMFC

The operation principle of a PEM fuel cell is presented in Fig.1. Humidified air enters the cathode channel and flows towards the catalyst. Hydrogen diffuses through the anode diffusion layer towards the catalyst (Heinzel *et al*., 1998; Biyikoglu, 2005). On the anode catalyst, hydrogen molecule splits up into two hydrogen protons and two electrons as follows:

$$2H_2 \rightarrow 4H^+ + 4e^-. \quad (1)$$

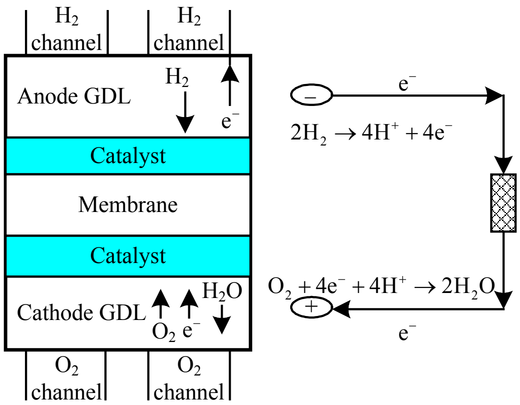

Fig.1 Operation principle of a PEM fuel cell

Electrons travel through an external circuit and then form a current, while protons migrate through the membrane.

On the cathode side the oxygen diffuses through the diffusion layer, splits up at the catalyst layer surface and reacts with protons coming from anode catalyst and electrons coming from external circuit according to:

$$O_2 + 4e^- + 4H^+ \rightarrow 2H_2O. \quad (2)$$

From the above, we can see that the overall reaction in a PEMFC can be written as:

$$2H_2 + O_2 \rightarrow 2H_2O \quad (3)$$

The voltage of a single cell is about 0.75 V. To obtain higher power, several cells are usually assembled into a PEMFC stack, where the cells are electrically connected in series and separated from each other by bipolar plates.

PEMFC system

Besides fuel cell stack, a fuel cell system needs to integrate several auxiliary components. Fig.2 is an example of a fuel cell system. The hydrogen supply valve reaching the desired flow or pressure is controlled by a valve. An air compressor supplies air. Anode and cathode gases have an external humidification system. A water cycle system removes the excess heat via a heat exchanger. Power conditioning is usually needed since the voltage of the fuel cell stack varies significantly and users also need various power sources. In this study, we assume that the stack is well designed so that all cells perform similarly. When abnormality occurs, every cell is represented by the same set of polarization curves. This assumption of invariable cell-to-cell performance is necessary for low-order-system models (Pukrushpan *et al*., 2005).

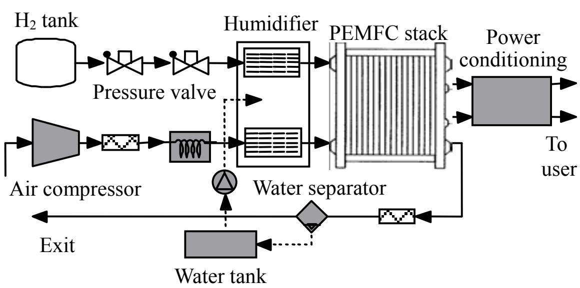

Fig.2 A fuel cell system example

FUEL CELL SYSTEM HYBRID MODEL

Brief introduction of ANN model

The basic unit of ANN is the artificial neuron. The neuron receives numerical information from input nodes, processes it internally, and outputs the result (Furrer and Thaler, 2005). The topology of the network is defined by the organization of the neurons. The most commonly used is the multilayer perception (MLP) type. In a feed forward architecture, the outputs of the layer are the inputs of the following one. First layer is called input layer. Last layer is called output layer. The layers between the input layer and the output layer are called hidden layers. An artificial neural network based PEMFC model has simple structure, concise algorithm, good convergence and great adaptability to the environment (Tian *et al.*, 2005). Lee *et al.*(2004) researched on a simulated 60 kW PEMFC cogeneration system for domestic application. They used a two-layered network with tangent hyperbolic activation function in hidden layer units, and a linear transfer function in the output unit to build a model of fuel cell, and obtained that the ANN model can simulate the experimental data for different operating conditions and hence can be used to investigate the influence of process variables. ANN also is successfully used in fuel cell system optimization and management (Ahmed and Istvan, 2005).

Rationale of Hybrid model

As known, too complex physical model, including empirical model and mechanical model, cannot be used in practice. But too simplified physical model is not enough to accurately represent a fuel cell system. So, it is urgent to develop a simple but sufficiently accurate PEMFC model for engineering applications (Marr and Li, 1998). In order to more accurately predict the performance of a PEMFC when only limitedly accurate physical model is available, Ou and Achenie (2005) proposed a hybrid model consisting of a physical component and a black-box component. The physical model has good stabilization while the ANN model has good accuracy in multi-dimensional mapping, so the one can be compensated by the other. The rationale behind this approach is to combine the part of the model that is well known from the physics of the problem with the part that is poorly known but can be estimated quite effectively by neural network. In the hybrid model, the ANN component only tackles the theoretically unknown parts and the other parts are already addressed by the physical component. From this way, we can save much experimental data and training time to achieve equivalent accuracy hybrid model.

The hybrid model schematic is shown in Fig.3 and the input-output relationship can be described as:

$$\boldsymbol{Y}=\boldsymbol{Y}_{\text{physical}}(x_1,x_2,\ldots,x_N)+\boldsymbol{Y}_{\text{ANN}}(x_1,x_2,\ldots,x_N). \quad (4)$$

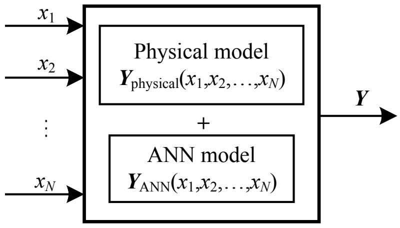

Fig.3 The schematic of hybrid model

The vector $\boldsymbol{X}=[x_1,x_2,\ldots,x_N]$, represents operating or design variables. The function $\boldsymbol{Y}_{\text{physical}}(x_1,x_2,\ldots,x_N)$ is a physical model with input $\boldsymbol{X}$. The function $\boldsymbol{Y}_{\text{ANN}}(x_1,x_2,\ldots,x_N)$ is an artificial neural network model with input $\boldsymbol{X}$ and approximates the unmodelled parts in the physical model.

The procedure to create a hybrid model is shown in Fig.4. Based on these experimental data, input $\boldsymbol{X}_{\text{experiment}}$ and output $\boldsymbol{Y}_{\text{experiment}}$ can be obtained. By input vector $\boldsymbol{X}_{\text{experiment}}$, the physical model can generate a simulated output vector $\boldsymbol{Y}_{\text{physical}}$. $\boldsymbol{Y}_{\text{experiment-physical}}$ is the difference of experimental output and physical model output. Using $\boldsymbol{X}_{\text{experiment}}$ (input data) and $\boldsymbol{Y}_{\text{experiment-physical}}$ (output data) as training data to train ANN model. $\boldsymbol{Y}_{\text{ANN}}$ is the output of ANN model. The target output of the hybrid model $\boldsymbol{Y}_{\text{hybrid}}$ is the summation of $\boldsymbol{Y}_{\text{ANN}}$ and $\boldsymbol{Y}_{\text{physical}}$.

In this study, the physical model comes from (Al-Baghdadi, 2005; Fazil and Serhat, 2005).

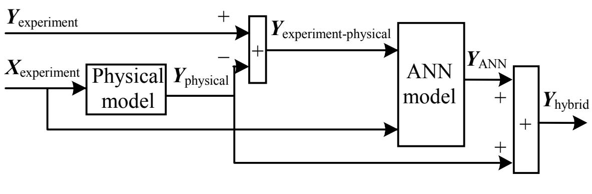

Fig.4 Hybrid model framework

The expression of the voltage of a single cell is:

$$V_{\text{cell}}=E+V_{\text{act}}+V_{\text{ohmic}}+V_{\text{diff}}$$
$$=E+\xi_1+\xi_2T+\xi_3T[\ln(C_{O_2})]+\xi_4T[\ln(i)]$$
$$-iR^{\text{internal}}-b\ln(1-i/i_{\max}), \quad (5)$$

where V_{cell} is single cell output voltage; E is the reversible thermodynamic voltage; V_{act} is activation overvoltage; V_{ohmic} is ohmic overvoltage, V_{diff} is diffusion overvoltage; T is cell temperature; C_{O_2} is oxygen concentration at the cathode membrane; i is current density; R^{internal} is total internal resistance; $i_{\max}$ is maximum current density.

The stack output voltage can be represented as:

$$V_{\text{stack}}=nV_{\text{cell}}, \quad (6)$$

where n is the number of fuel cells.

In the stack model, empirical coefficients can be obtained by a fitting procedure based on the measured polarization curve of the stack. The parameters of this stack model are given in Table 1.

Table 1 Parameters of PEMFC stack

Model parameter	Value
ξ_1	−0.9514
ξ_2	0.00312
ξ_3	7.4×10^{-5}
ξ_4	-1.87×10^{-4}
b (V)	0.02027454
$i_{\max}$ (mA/cm^2)	430

The input variables of ANN model include current density, reactant pressures, stoichiometry and temperature. The output variables can include output voltage, efficiency, power density and net power density. The factors affecting the network's hidden layer neurons are the number of samples in a training set, the noisy extent of samples and the complexity degree of function or classification to learn (Yuan *et al*., 2003). Although it is very difficult to effectively decide the number of hidden neurons, there is an optimal number of hidden neurons. An optimal number of hidden neurons need to be determined for each neural network to achieve the best performance and can be obtained by trial and error. Fig.5 shows that the training is based on different numbers of hidden neurons and that the MSE curve is the minimum mean square error of the target output value in the network stabilization. Therefore, 19 neurons of the hidden layer are determined under synthetic consideration of the performance and the efficiency.

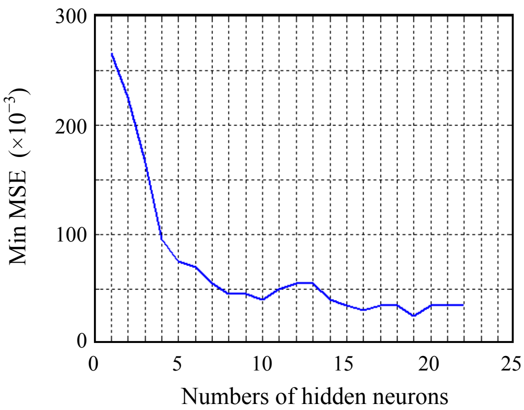

Fig.5 Convergence curves of network training on different hidden neurons

VALIDATION OF THE HYBRID MODEL

Model validation involves the comparison of model results with experimental data, physical model results and ANN model.

Fig.6 is the compared results among the hybrid model, physical model and the experimental data at general operating temperatures (Shan and Choe, 2005). The experimental data used in this study came from the Institute of Fuel Cell, Shanghai Jiao Tong University. We can see that the estimated results of hybrid model are much better than those of the physical model. So, the hybrid model can be applied to predict fuel cell output voltage more accurately. That is because of the limitation of many currently available physical model parameters. The choice of model parameters may significantly affect the characteristics of the simulated model. The parameters values are either based on manufacturing data or based on laboratory experiments (Correa *et al*., 2005). Many parameters, such as semi-empirical coefficients, mass transfer coefficients and intrinsic rate constant, of physical model have to fit experimental data. After validation, those parameters are fixed and cannot adapt new operating conditions. The hybrid model can obtain better-simulated results because it uses ANN component to compensate the aforementioned shortage of the physical model.

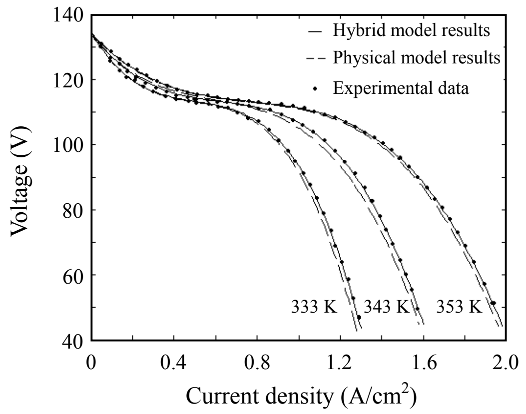

Fig.6 Comparison between hybrid model and experimental data

Lee *et al.*(2004) proposed more careful analyses of the ANN model by varying the process variables and obtained results showing that fuel cell stack output voltage is proportional to gas pressure. From Fig.7, we can have the similar curves.

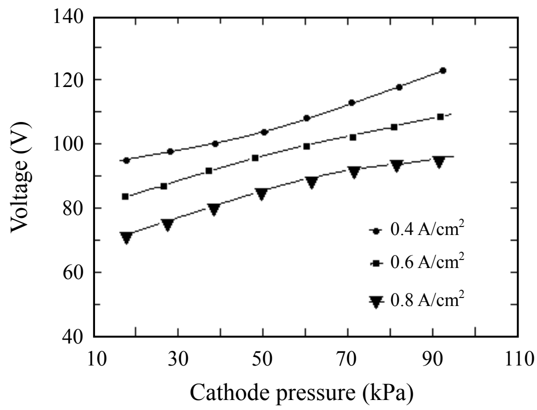

Fig.7 Effect of cathode pressure on stack voltage for different current density

Fig.7 shows the variations of stack voltage with reactant gas pressure when current densities are 0.4, 0.6 and 0.8 A/cm^2. Cathode gas pressure is a little more than anode gas pressure for avoiding hydrogen osmosis. The remaining variables were regulated at values of stack temperature 80 °C, stack inlet temperature 80 °C, and membrane humidity 100%. When current density was set constant, the stack voltage is proportional to cathode pressure.

Fig.8 shows the performance comparison of hybrid model and ANN model at different operating conditions. Input variables include discharge current, inlet reactant temperatures, relative humidity values, gas pressures, gas utilities, and cell temperature. The simulated results by hybrid model agreed well with the experimental data. The hybrid model results are slightly better fitting experimental data than those of ANN model. So, when the experimental data are inadequate, we can use the hybrid model to substitute for the ANN model to improve the model performance.

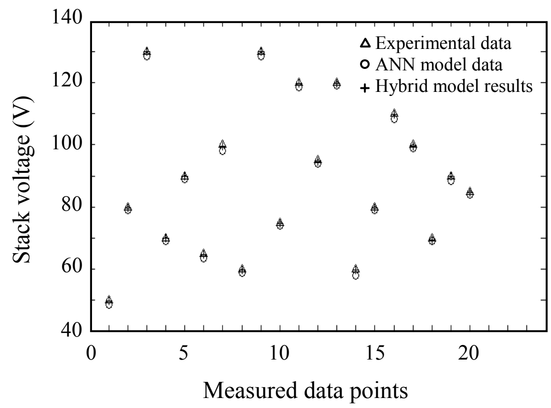

Fig.8 Comparison of hybrid model to ANN model and experimental data

Table 2 gives a more direct description of simulation results. The maximum voltage estimation error of physical model is 0.45% while that of hybrid model is 0.27%. Besides fuel cell stack model, a complete system also includes many subsystems, such as fuel and air supply, water management, heat management and a power conditioning system (Pathapati *et al.*, 2005). The hybrid model is used as a subsystem of a total fuel cell system. A higher pressure of the stack leads to a higher power, but a higher pressure also leads to a higher parasitic power. The shifting trend of the power density curve is opposite to that of the efficiency curve. So, there is a tradeoff between high power and high efficiency. The maximum net power density is 39.569 W/cm^2 when the current density is 1.2 A/cm^2, not at the maximum efficiency point or at the maximum power point.

Table 2 Simulation results

Current density (A/cm^2)	Experimental voltage (V)	Physical model voltage (V)	Hybrid model voltage (V)	Efficiency	Power density (W/cm^2)	Net power density (W/cm^2)
0.1	108	107.855	107.962	0.69	10.796	7.449
0.2	101	100.872	100.963	0.65	20.192	13.125
0.3	97	96.825	96.937	0.62	29.081	18.030
0.4	94	93.815	93.941	0.60	37.576	22.546
0.5	91	90.828	90.951	0.57	45.476	25.921
0.6	89	89.052	89.013	0.55	53.408	29.374
0.7	86	86.041	86.005	0.53	60.204	31.908
0.8	84	83.872	83.995	0.51	67.196	34.270
0.9	82	81.855	81.904	0.50	73.714	36.857
1.0	80	79.872	79.935	0.47	79.935	37.569
1.1	78	77.854	77.948	0.46	85.743	39.442
1.2	75	74.831	74.942	0.44	89.930	39.569
1.3	72	71.801	71.925	0.42	93.503	39.271
1.4	70	69.809	69.905	0.40	97.867	39.147
1.5	67	69.801	69.890	0.37	104.835	38.789
1.6	63	62.799	62.885	0.35	102.216	35.776
1.7	59	58.784	58.874	0.32	101.788	32.572
1.8	54	53.755	53.850	0.27	96.930	26.171

CONCLUSION

In this paper, a hybrid model is presented which comprises physical component and ANN component. Conventional physical model strategies have difficulties in parameters calculation. Non-parametric model, such as ANN model, provides an interesting and powerful solution without extensive calculation. But training ANN model needs too much time and experimental data. In order to obtain sufficiently accurate model in case that only limited accuracy physical models are available, a hybrid model was proposed. The motivation is that to improve the model performance, no sufficiently accurate physical models can be compensated by the ANN model. The simulated results showed that the hybrid model is more accurate than physical models and ANN models.

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