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Nonlinear modeling of PEMFC based on neural networks identification*

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Abstract: The proton exchange membrane generation technology is highly efficient and clean, and is considered as the most hopeful "green" power technology. The operating principles of proton exchange membrane fuel cell (PEMFC) system involve thermodynamics, electrochemistry, hydrodynamics and mass transfer theory, which comprise a complex nonlinear system, for which it is difficult to establish a mathematical model. This paper first simply analyzes the necessity of the PEMFC generation technology, then introduces the generating principle from four aspects: electrode, single cell, stack, system; and then uses the approach and self-study ability of artificial neural network to build the model of nonlinear system, and adapts the Levenberg-Marquardt BP (LMBP) to build the electric characteristic model of PEMFC. The model uses experimental data as training specimens, on the condition the system is provided enough hydrogen. Considering the flow velocity of air (or oxygen) and the cell operational temperature as inputs, the cell voltage and current density as the outputs and establishing the electric characteristic model of PEMFC according to the different cell temperatures. The voltage-current output curves of model has some guidance effect for improving the cell performance, and provide basic data for optimizing cell performance that have practical significance.

Key words: Proton exchange membrane fuel cell, Nonlinear system modeling, LMBP algorithm
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INTRODUCTION

With worldwide increase of air pollution and the environmental consciousness of governments, people have to look for new resources to mitigate the energy crisis and improve the present environmental status (Ferng *et al*., 2004; Rowe and Li, 2001). Fuel cells are highly efficient and environmentally clean electrical generators (Mann *et al*., 2000) that convert the chemical energy of a gaseous fuel directly into electricity energy and play an important role in solving the problem of energy and traffic. Therefore worldwide attention has been focused on the development of fuel cells which will become alternative energy resources in the future (Bender *et al*., 2003). A fuel cell system can yield overall efficiency of up to 80% and net electrical efficiency of 40% to 60%, which are higher than that of almost all other energy conversion systems (Baschuk and Li, 2000). Among five different kinds of fuel cells, the proton exchange membrane fuel cell (PEMFC) has advantages of low operational temperature (20 °C~100 °C), little noise, rapid startup, high power density and light weight, and turns into the investigative focus of fuel cells (Berning and Djilali, 2003). PEMFC is being applied to vehicle power systems, portable electrical resources and distributed power generation (such as district power station, family power supply) successfully and is considered as the most promising fuel cell technology in the future.

PEM FUEL CELL SYSTEMS

The typical structure of a single PEMFC is shown in Fig.1. A single cell consists of anode, cathode, electrolyte plate and current collectors with

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gas channels. H_2 and O_2 get through the gas channels of currents collectors and arrive at the anode and cathode respectively; the reactive gases pass the diffusion layer and reach the proton exchange membrane (50~170 μm thick). On the anode side, the hydrogen splits into hydrogen protons and electrons under the action of the catalyst, and the hydrogen protons pass through the polymer electrolyte membrane under the action of electricity. On the cathode, the oxygen diffuses towards the catalyst interface where it combines with the hydrogen protons and the electrons to form water, as pointed out by Berning *et al.*(2002). The electrons passing from anode to cathode produce electrical energy.

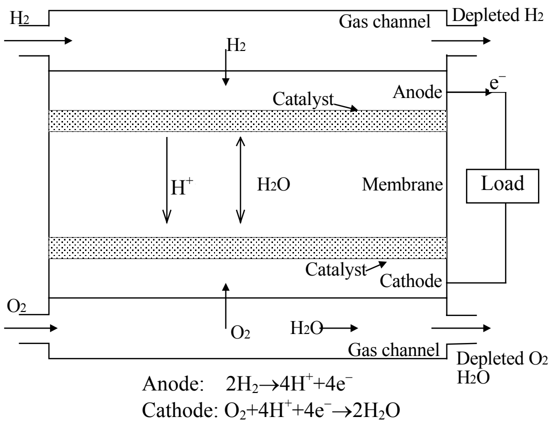

Fig.1 Schematic of a PEM fuel cell

In the past decades, the researches on PEMFC are mainly focused on the structural design of a single cell, catalyst layer and gas diffusion layer, the manufacture of high performance membrane and catalyst, the thermal and water management of PEM fuel cells. The researchers investigated deeply the components and PEMFC system. Different static and dynamic models of PEMFC have been established on the basis of the energy, mass and momentum conservation laws. The components and single cell model were founded based on the operational mechanism, and research was carried out on the working parameters (gas flow rate, pressure, humidity, cell temperature and moisture content) affecting the output voltage. But the large number of experimental parameters in the models of components and single cell lead to overall decrease in performance. Moreover, the hypothetical and simplified conditions in modeling cause the precision to decline greatly; and the expressions of model are so complex that it is difficult to apply them in the design of PEMFC system.

The stack of PEMFC is made up of 32 cells (active area 128 cm^2) and can supply electrical power up to 1 kW at 24 V. The catalyst P_t and Nafion112 are used to prepare MEA (membrane electrode assembly). The operating temperature ranges from 20 °C to 100 °C. The stack of PEMFC is shown in Fig.2.

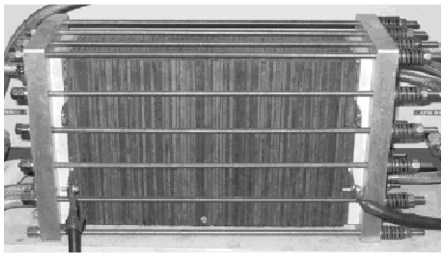

Fig.2 PEM fuel cell stack

The generation of electricity by the proton membrane fuel cell is influenced by several factors. Accurate test of the PEMFC system contributes to understanding the generating electricity characters and controlling the various parameters which make the system operate in the optimum status. And we gathered the several groups of experimental data from it as the training samples of the neural networks. The map of test bench is shown in Fig.3.

Fig.3 Photograph of the test equipment

In order to improve the reliability, stability and life-span of PEMFC system, it is essential to establish the dynamic model and carry out the real time control. Water content in membrane and operating temperature greatly affect the performance of the output voltage-current. The method of neural network was adopted by Shen (2002) and Shen and Cao (2002) to control the optimal operating temperature of molten carbonate fuel cell. The range of temperature for stable PEMFC operation is about 20 °C~100 °C, and the optimal operating temperature is about 80 °C. Higher operating temperature is favorable for the rate of electrochemistry reaction and the transfer speed of proton in the proton exchange membrane; on the other hand, the higher operating temperature accelerates loss of water in the membrane, and lead to decrease performance of the membrane and cells. Consequently, the appropriate range of temperature is key to improving the performance and prolonging the life-span of cells.

NEURAL NETWORK IDENTIFICATION ALGORITHM

Feedforward neural networks trained with the back propagation (BP) algorithm, have been widely used in system identification and control. BP neural network consists of three main parts. The first part is the input layer which distributes the input data to the processors in the next layer. The second part is made up of hidden layers where the nonlinear behavior comes from. The third part is the output layer which transmits the response of the network to the real world. Input and output layers are directly accessible while the hidden layers are not. Each layer contains several processing elements which are generally called neurons and were introduced by Efe *et al.*(1999). The BP network structure is shown in Fig.4. x_1, x_2, …, x_m denote the inputs of the network, y_1, y_2, …, y_r denote the hidden units, and O_1, O_2, …, O_P denote the outputs of the hidden layer units. The connections between the units of different layers are called weight and bias. The output training data are referred to as the target output of the neural network. The goal is to train the network until the output of the neural network is suitably close to the target output, as pointed out by Kalogirou (2001).

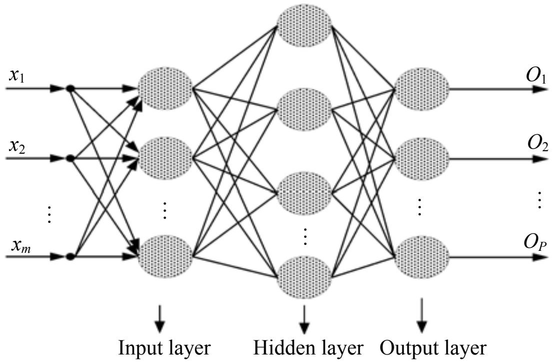

Fig.4 Structure of the BP network model

We define the error of the *P*th sample as follows, where t_{pi}, O_{pi} denote the desired output and network computing output, respectively. For this purpose, the value of the following equation must be minimized. P is the total number of training pairs included in the training data set and N is the number of the neural network outputs.

$$E_P = \frac{1}{2}\sum_{i}^{N}(t_{pi} - O_{pi})^2 \tag{1}$$

The BP network learning method is to make the error function down the direction of the negative gradient for correcting the weight and bias of the network. Considering the forward pass through the network, for a set of input values, the output of the ith hidden layer unit is given by

$$y_i = f(\sum_i w_{ij}x_j - \theta_i) \tag{2}$$

where f is the activation function, w_{ij} is the weight of connection from ith input unit to the jth hidden layer unit, and θ_i is the bias value of the jth hidden layer unit. And the output is given by

$$O_i = f(\sum_i w_j x_j - \theta) \tag{3}$$

where w_j is the strength of the connection from the jth hidden layer unit to the output unit, and θ is the bias value of output unit (Lee *et al.*, 2004). The change in weight Δw_{ij} is based on the gradient descent and is given by

$$\Delta w_{ij} = -\eta \frac{\partial E}{\partial w_{ij}} \tag{4}$$

where η is the learning rate.

The neural network has the ability to learn and approach the nonlinear function, which has been considered as a powerful computing tool for establishing the mathematical relationship of the dynamic system based on the input-output data. At present, BPNN (Back-Propagation Neural Network) has been used extensively in the areas of system modeling, pattern recognition and function approach. But BPNN has its limits and shortcomings, such as the long training time and the local least value. Accordingly, we adopt the Levenberg-Marquardt BP algorithm, and establish the PEMFC model; then use the testing data as the training samples. On the condition of the enough hydrogen, considering the air (oxygen) flow rate and the inlet cooling water temperature as the input of model, the cell voltage and current density as the output of the model. The PEMFC electro-chemical character models are eventually established for different working temperatures after learning and training.

The voltage and current density characters can be described on the basis of the analysis of dynamic PEMFC system as:

$$U(t) = \phi[U(t), I(t), T(t), V] \tag{5}$$

$$I(t) = f[U(t), I(t), T(t), T] \tag{6}$$

Voltage of a single cell is about 0.8 V and current density is approximately 300~800 mA/cm^2. To supply higher power, cells are usually arranged into a PEMFC stack, where the cells are electrically connected in series and separated from each other by bipolar plates (Kumar and Reddy, 2003). The PEMFC stack test system illustrated in Fig.5 includes cells, fuel cycle system, oxidant cycle system, water and thermal management system. The fuel and oxidant cycle system mainly provides the PEMFC stack with fuel and oxidant. The water and thermal management system mainly ensure the balance of water/temperature in the stack and maintain the optimum working condition, as discussed by Wang *et al*.(2003), Maggio *et al*.(2001) and Rodatz *et al*.(2004). In order to guarantee the cells' normal operation, the control system must manipulate the inlet gas flow rate and the inlet cooling water flow rate so that they accord with the requirement that the power of the cells must match the variation of the load, and the change of cells working condition. Regulating the cooling water flow rate and collecting the groups of output voltage/current density values of the cell at 40 °C, 60 °C and 80 °C of working temperature respectively. The test data are shown in Table 1.

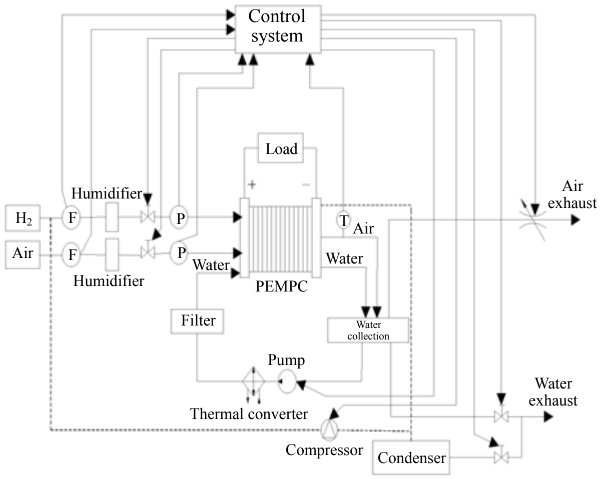

Fig.5 PEMFC generation system

This paper puts forward the modeling method of neural network by utilizing the experimental data to avoid the complexity of PEMFC generation system.

The model should simulate the cell polarization curve at different temperatures, as well as complete the dynamic nonlinear map from input vector to output vector. The identification model can be described by the nonlinear differential equation:

$$U(k+1) = \phi[U(k), I(k), T(k), V] \tag{7}$$

$$U(k+1) = \phi[U(k), I(k), T(k), V] \tag{8}$$

IDENTIFICATION STRUCTURE AND ALGORITHM OF PEMFC SYSTEM

The PEMFC system identification structure is

Table 1 The output voltage/current test data of PEMFC

I (A/cm^2)	0	0.015	0.025	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1	1.1	1.2
U (40 °C)	1.05	0.90	0.82	0.77	0.73	0.69	0.65	0.61	0.57	0.54	0.50	0.46	0.42	0.37	0.32
U (60 °C)	1.05	0.90	0.82	0.77	0.73	0.70	0.66	0.63	0.60	0.57	0.54	0.51	0.48	0.45	0.42
U (80 °C)	1.05	0.90	0.82	0.78	0.76	0.74	0.72	0.70	0.68	0.66	0.64	0.62	0.59	0.55	0.52

shown in Fig.6, TDL denotes a tapped delay line whose output vector acts as the delayed values of the input signal so that past values of the input and output of the system from the input vector to a neural network whose output $\hat{U}(k+1)$ corresponds to the estimation of the system output at any instant k. Since the above model has no feedback loop, training procedures can be used to adjust the parameters.

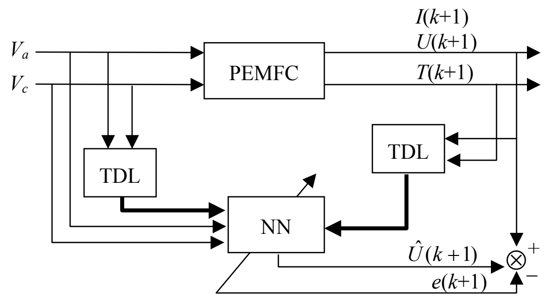

Fig.6 Identification structure of PEMFC system

We adopt the feedforward BP neural network including a hidden layer which has 20 nerve units. Sigmoid function should be taken as the transfer function, whose expression is $2/(1+\exp(-2n))-1$, and the error function as expressed lay the squared deviation. The dynamic response value should be considered as training sample at the three different temperatures, and should be saved in the data training file which should be provided the network during its training. Since BP neural network usually has low training speed, and easily gets into minimum value, so the BP algorithm cannot strictly assure the convergence and optimum in training. Therefore we adopt the Levenberg-Marquardt BP algorithm to train the network. The Levenberg-Marquardt algorithm is a Newton algorithm, which uses Hessian inverse matrix in place of the product of learning ratio multiplied by the decreasing direction of error gradient, where Hessian matrix is the error index for the second derivative of current weight, and quadratic function is used to approach the objective function at the adjacent extreme points. Accordingly, the rate of Newton algorithm convergence is faster than that of the generic BP algorithm. The regulating weight equation of the Levenberg-Marquardt algorithm is as follows:

$$x^{k+1} = x^k + (\boldsymbol{J}^{\mathrm{T}}\boldsymbol{J} + \mu\boldsymbol{I})^{-1}\boldsymbol{J}^{\mathrm{T}}e \qquad (9)$$

where $\boldsymbol{J}$ is Jacobian matrix which is the differential error for the weight value, the term which includes $\boldsymbol{J}^{\mathrm{T}}\boldsymbol{J}$ can be neglected, so that the process of learning accords mainly with $\boldsymbol{I}^{-1}\mu^{-1}\boldsymbol{J}^{\mathrm{T}}e$. The learning property of the algorithm should be decided by μ which is an adaptive adjusting scalar. If the error increases, the value of μ would also increase, and the process of learning mainly accords with the gradient descent algorithm, otherwise the value of μ approach to zero, the process of learning mainly accords with the Gauss-Newton algorithm. The dynamic variation of μ can assure decrease error at each step.

IDENTIFICATION RESULT OF PEMFC SYSTEM BASED ON NN

Dynamic identification of the PEMFC system should be carried out by simulation using neural network which had been trained (Table 2).

In the experiment, PID control method was adopted to adjust the flow rates of anode and cathode inlet gas. The variation value of voltage/current calculated by the neural network compared favorably with the actual value. The identification curve is shown below.

During the training process, the error curve variation under different temperatures is shown in Fig.8. Fig.7 shows that the error is 0.00098 less than the goal error of 0.01 set in the program. The performance of the network meets the requirement. The neural network model can simulate the dynamic response of voltage/current, and the maximal error is less than 0.002 V. The training error is decided by the goal error, choosing the most suitable neural network to improve the accuracy of identification with the

Table 2 Operating conditions of PEMFC

Item	Value
Fuel gas	H_2/H_2O=0.86/0.14
Relative humidity	100 %
Electrode thickness	0.3 mm
Membrane thickness	0.13 mm
Current collector thickness	4 mm
Cathode pressure	2.5 atm
Anode pressure	2.5 atm
Cathode gas flow rate	4.5 L/min
Anode gas flow rate	2.4 L/min
Humidification temperature	70 °C
Hydrogen inlet temperature	65 °C
Oxygen inlet temperature	80 °C
Inlet cooling water temperature	70 °C
Active area of cell	128 cm^2

method of trial and error. 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. But measures should be adopted to prevent the disadvantages of dehydration of membrane and increase of vapour partial pressure.

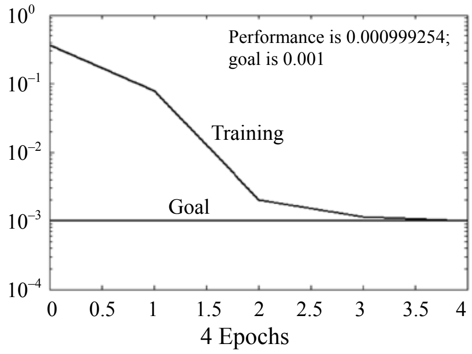

Fig.7 Learning error of LMBP algorithm

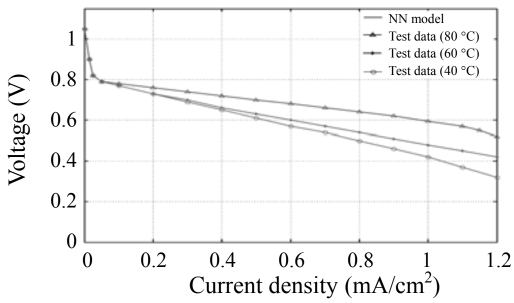

Fig.8 Polarization curves for different cell temperatures

However, the Levenberg-Marquardt BP algorithm requires a large amount of storage space, because the Jacobian matrix uses a $Q*n$ matrix, where Q is the number of training samples and n is the total number of weight and bias in the network. In most cases, this algorithm can achieve relatively good result, but the conclusion is not supported by relevant theory, so different initial values should be trained several times for the network. Furthermore, we can use other global optimization algorithm, such as simulated annealing algorithm and genetic algorithm.

CONCLUSION

The simulation results showed that the proposed LMBP neural network can be feasibly set up to model the complex nonlinear PEMFC system with relatively highly modeling accuracy. At the same time, it avoids the complex calculation of the modeling by mechanism and reflects the dynamic behavior of PEMFC output voltage/current and provides a basic guide for design and analysis of the PEMFC power system and the optimization of cell performance.

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