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基于改进 RBFNN 的 SOFC 辨识建模

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摘 要 针对现有的固体氧化物燃料电池(SOFC)模型过于复杂,难以满足控制系统的设计需要的弊端,基于一种改进的径向基函数神经网络(RBFNN)辨识技术建立了 SOFC 的非线性模型。在建模过程中,以 SOFC 的燃料利用率为模型的输入,电压和电流为模型输出。利用 800 组实验数据作为训练样本,建立了 SOFC 的电流-电压辨识模型。仿真结果表明了所建模型的有效性和精度。该模型的建立为先进的控制策略研究奠定了基础。

关键词 固体氧化物燃料电池(SOFC) 径向基函数神经网络(RBFNN) 建模 辨识

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Solid oxide fuel cell (SOFC) is an energy conversion device that produces electricity by electrochemically combining fuel (*e. g.*, hydrogen) with oxidant (*e. g.*, oxygen) gases across an ionic conducting oxide[1]. The SOFC operates at relatively high temperatures (800 ℃ ~1 000 ℃) under atmospheric or elevated pressures, depending on the fuel cell design and intended use. Under typical operating conditions, single cells (each cell producing less than 1V) are stacked to produce the required power and voltage levels. Because of all solid-state construction, the SOFC can be made into compact and lightweight units for increased power densities. The key feature of this fuel cell technology is its clean and efficient generation of electricity from a variety of fuels[2].

An important tool in the fuel cell development is mathematical modeling, which has the capability of predicting the fuel cell performance. It is well known that SOFC is sealed, and work at high-temperature and in a complicated environment. SOFC is a nonlinear system with multi-input and multi-output, and it is very difficult to model using the traditional methodologies. In last several decades, many SOFC stack models have been reported[3—5]. However, most of the existing models developed are based on mass, energy and momentum conservation laws, and their expressions are too complicated to meet the demand of control system design for the SOFC.

Neural network is considered as an attractive structure to establish the mathematical relationship of the dynamic system based on the input-output data. It has been shown that feed-forward neural networks with one hidden layer can uniformly approximate any continuous function to a specified accuracy. In this paper, a kind of radial basis function neural network (RBFNN) based on orthogonal least squares (OLS) method is firstly proposed. Then, the authors try to avoid the internal complexity of the SOFC, a current-voltage identification model under different fuel utilizations is presented. The validity of the model is proved by simulation experiments.

1 Description and analysis of SOFC stack

A SOFC consists of an interconnect structure and

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a three-layer region composed of two ceramic electrodes, anode and cathode, separated by a dense ceramic electrolyte (often referred to as the PEN—Positive-Electrode/Electrolyte/Negative-Electrode). SOFC can use hydrogen, carbon monoxide and hydrocarbons as fuel, air (or oxygen) as oxidant. A typical H_2—H_2O, Ni | YSZ | Pt, O_2 fuel cell is shown in fig. 1. The principle of SOFC is based on the conversion of the chemical energy, which is stored in the fuel (hydrogen or methane), into electrical energy through an electron-producing electrochemical reaction. The detail process is as follows: 1) oxygen diffuses through the porous cathode material; 2) oxygen molecules are dissociated and ionized at the cathode/electrolyte interface; 3) oxygen ions migrate through the electrolyte towards the anode/electrolyte interface; 4) fuel diffuses through the porous anode material; and 5) hydrogen contained in (and/or produced by) the fuel reacts with oxygen ions, producing water and liberating electrons, that flow back to the cathode/electrolyte interface, via an external circuit[6].

To produce a useful voltage, a complete SOFC system can not be made up of a single solid oxide fuel cell, as its voltage is quite small (about 0.7 V when drawing a useful current), but most consist of several repeating electrochemical cells in a module, connected both in series and/or in parallel and assembled to compose a stack.

1.1 Physical model of the SOFC

The fundamental electrode reaction in the SOFC is different from that of other kinds of FC[7]. When using hydrogen as fuel, the electrochemical reactions of the SOFC at the anode and cathode, respectively, are

$$\text{Anode}: H_2 + O^{2-} \longrightarrow H_2O + 2e^- \tag{1}$$

$$\text{Cathode}: \frac{1}{2}O_2 + 2e^- \longrightarrow O^{2-} \tag{2}$$

To calculate the open-circuit emf of a stack of N_0 cells in series, refer to the well-known Nernst equation

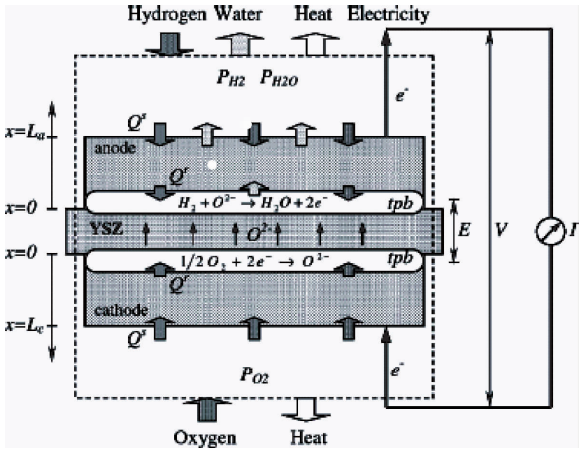

Fig. 1　Principle of SOFC

$$E = N_0E_0 + E_f\ln\left(\frac{p_{H_2}p_{O_2}^{0.5}}{p_{H_2O}}\right) = V_{dc} + rI_{FC} \tag{3}$$

Under steady state, the reaction output partial pressures are[8]:

$$p_{H_2} = (N_{H_2}^{in} - 2K_rI_{FC})/K_{H_2} \tag{4}$$

$$p_{H_2O} = 2K_rI_{FC}/K_{H_2O} \tag{5}$$

$$p_{O_2} = (N_{H_2}^{in}/r_{H\_O} - K_rI_{FC})/K_{O_2} \tag{6}$$

One factor not shown explicitly in the above model is the fuel utilization u. It is one of the important operating variables that may affect the performance of *FC*. Fuel utilization (u) is defined as follows:

$$u = \frac{N_{H_2}^{in} - N_{H_2}^{out}}{N_{H_2}^{in}} = \frac{N_{H_2}^{r}}{N_{H_2}^{in}} = \frac{2K_rI_{FC}}{N_{H_2}^{in}} \tag{7}$$

For protecting SOFC stack, the desired range of u is from 0.7 to 0.9. An overused-fuel condition ($u > 0.9$) could lead to permanent damage to the cells due to fuel starvation whereas an underused-fuel condition ($u < 0.7$) results in unexpectedly high cell voltages [9].

In this paper we only consider ohmic loss, i. e.

$$V_{dc} = E - rI_{FC} \tag{8}$$

From eq. (3) – Eq. (8), the terminal voltage of the SOFC is:

$$V_{dc} = N_0E_0 + \ln\left[\frac{K_{H_2O}}{K_{H_2}}\left(\frac{K_r}{r_{H\_O}K_{O_2}}\right)^{0.5}\right]E_f - rI_{FC} + \frac{1}{2}\ln\left[I_{FC}\left(\frac{1}{u}-1\right)^2\left(\frac{2}{u}-r_{H\_O}\right)\right]E_f \tag{9}$$

where, E_0 is the voltage associated with the reaction-free energy of a cell, N_0 is the number of series cells in the stack, $E_f = N_0RT/2F$, R is the gas constant, T is the SOFC operating temperatures, F is the Faraday constant, p_i are the partial pressures of hydrogen, oxygen, and water. r_{H_O} is the ratio of hydrogen to oxygen molar flows. $N_{H_2}^{in}$, $N_{H_2}^{out}$, and $N_{H_2}^{r}$ are hydrogen input, output and reacted flow rates. K_r is a modeling parameter which has a value of $N_0/4F$. K_i are the valve molar constant of hydrogen, oxygen, and water. r is ohmic loss. Some of the above parameter values are given in table 1.

Table 1 Parameters of the SOFC stack

Symbol	Value
T	1 273 K
E_0	1.18 V
N_0	384
K_r	0.993×10^{-3} mol/(s. A)
K_{H_2}	0.843 mol/(s. atm)
K_{H_2O}	0.281 mol/(s. atm)
K_{O_2}	2.52 mol/(s. atm)
r	0.126 Ω
r_{H_O}	1.145

The fuel cell stack's performance, voltage-current model under the steady state is shown as eq. (9). But this model is too complexity to be used in the control system design. To develop effective control strategies, it's necessary to establish an identification model of the SOFC suitable for control system design.

2 Description of the improved RBFNN

Recently, RBFNN is increasingly employed in a wide range of applications because of its mighty and rapid local approximate ability. But there exist two bottleneck problems, i. e., how to select the appropriate centers in the hidden layer and the output layer weights. OLS method is one of the valid methods to settle the above two problems in RBFNN[10].

Without loss of generality, we assume RBF output layer has one neuron. Provided that the training sample pairs of network are $\{X_n, d(n)\}$ $(n = 1, 2, \cdots, N)$, N is the number of training sample pair; X_n is the input data vector; $d(n)$ is the desired output response of the network. According to the linear regression model, the desired output response of the network can be expressed:

$$d(n) = \sum_{i=1}^{M} p_i(n) w_i + e(n) \tag{10}$$

where, M is the number of neuron in hidden layer, and also is known as the number of network center, $M \leqslant N$; w_i is model parameter which is the connect weight between output layer and hidden layer; $e(n)$ is residual error; $p_i(n)$ is regression operator which in fact is the response of network center under some basis function $\Phi(\cdot)$. Here $\Phi(\cdot)$ is the Gaussian function.

The eq. (10) can be written as the following matrix equation:

$$d = PW + e \tag{11}$$

where

$d = [d(1), d(2), \cdots, d(N)]^{\mathrm{T}}$,

$P = [P_1, P_2, \cdots, P_M]$,

$P_i = [P_i(1), P_i(2), \cdots, P_i(N)]^{\mathrm{T}}$ $(1 \leqslant i \leqslant M)$,

$W = [W_1, W_2, \cdots, W_M]^{\mathrm{T}}$,

$e = [e(1), e(2), \cdots, e(N)]^{\mathrm{T}}$.

Using the orthogonal decompose and least square algorithm, contribution ratio of orthogonal vector u_i to decreasing output error is defined as:

$$[e_r]_i = \frac{g_i^2 u_i^{\mathrm{T}} u_i}{d^{\mathrm{T}} d}, 1 \leqslant i \leqslant M \tag{12}$$

The appropriate regression operator subset can be found simply and availably using Gram-Schmidt orthogonal decompose method by eq. (12), and at the same time the RBF nerve centers and connect weights can be determined.

When $1 - \sum_{j=1}^{M_s} [e_r]_j < \rho$ (ρ is allowable error threshold specified) come into existence, the iterative ends up. By now the $N \times M_s$ orthogonal matrix U composed of M_s orthogonal vectors and corresponding triangular matrix A are known. Then the weight matrix W can be calculated from $g = AW$. And the set of center points is no other than the same subscript chosen during the orthogonal decompose (namely the training sample set with the subscript $i_1, i_2, \cdots, i_{M_s}$).

3 Identification model of the SOFC stack with improved RBFNN

The identification structure of the SOFC stack is shown in fig. 2. TDL is the tapped delay line, and the predictive error $e(n) = d(n) - y(n)$. In this paper, the training criterion of RBFNN is to minimize the mean square errors (MSE) below

$$E_{\mathrm{MSE}} = \frac{1}{N} \sum_j \sum_n (\mathrm{d_j}(n) - \mathrm{y_j}(n))^2 \qquad (13)$$

where, N is the number of data, $d(n)$ and $y(n)$ denote the desired and model outputs. Actually, the desired $d(n)$ is the experimental data.

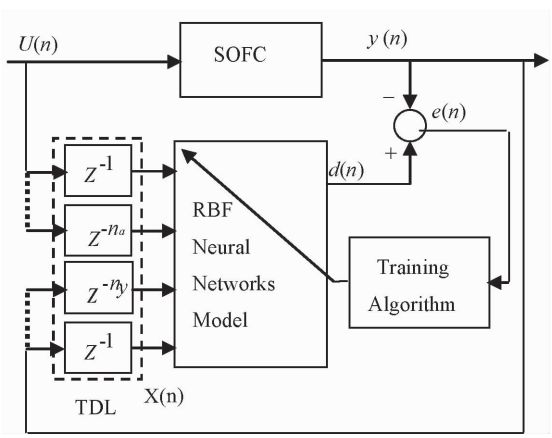

Fig. 2　Identification structure of the SOFC stack with RBFNN

Training of the RBFNN can be divided into two-stage procedures. The first stage is to ascertain the centers in the hidden layer and the output layer weights. The second is to train the network using training data to produce the correct output.

Here, the RBF network is trained using 800 groups of experimental data. The fuel utilization of SOFC is taken as the input and the voltage and current density as the output of the neural network model. Once the RBF network provides a satisfactory output on the validation data, cross-validation is carried out with test sample (200 groups of experimental data). After this final test, the network is ready to generate I-V characteristics for a broad range of conditions.

4 Results

The current-voltage characteristics at different fuel utilizations by the RBFNN model show good consistency with the experimental data, as shown in fig. 3.

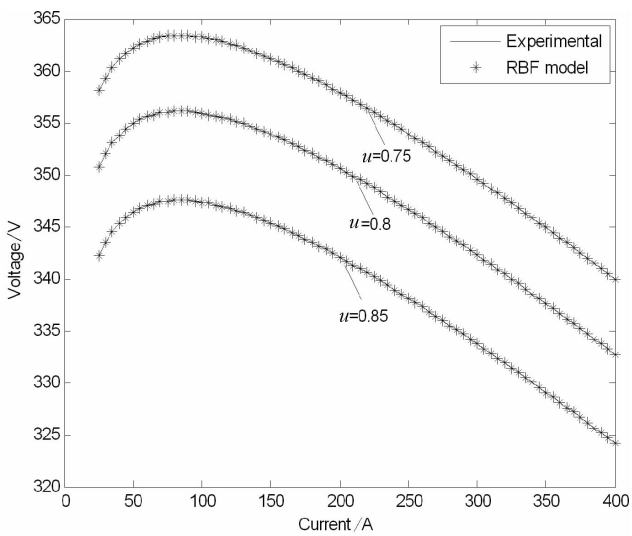

Fig. 3　Voltage-current characteristic: predicted by RBFNN model and experimental at different utilizations

From fig. 3, we can observe that the cell voltage decreases with increasing fuel utilization. This is because the Nernst potential has a greater decrease at greater fuel utilizations due to the enhanced depletion of reactant partial pressures. The simulation results show

the validity and accuracy of the model. The RBFNN identification model established in this study makes it possible to design on-line controller of the SOFC.

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Modeling SOFC Based on Improved RBFNN Identification

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[**Abstract**] According to the drawbacks of the existed mathematic models, which are too complicated to meet the design demand of SOFC control system, a nonlinear model based on a kind of improved RBF neural network (RBFNN) identification technique is presented. The fuel utilization of the SOFC is taken as the input, the voltage and current density as the outputs of the neural network model. With 800 groups of experimental data as the training samples, a cell voltage and current density identification model of the SOFC is established. The simulation results show the validity and accuracy of the model. Furthermore, based on this RBFNN identification model, some advanced control schemes can be developed.

[**Key words**] solid oxide fuel cell (SOFC) radial basis function neural network (RBFNN) modeling identification