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Nonlinear modelling of a SOFC stack by improved neural networks identification

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Abstract: The solid oxide fuel cell (SOFC) is a nonlinear system that is hard to model by conventional methods. So far, most existing models are based on conversion laws, which are too complicated to be applied to design a control system. To facilitate a valid control strategy design, this paper tries to avoid the internal complexities and presents a modelling study of SOFC performance by using a radial basis function (RBF) neural network based on a genetic algorithm (GA). During the process of modelling, the GA aims to optimize the parameters of RBF neural networks and the optimum values are regarded as the initial values of the RBF neural network parameters. The validity and accuracy of modelling are tested by simulations, whose results reveal that it is feasible to establish the model of SOFC stack by using RBF neural networks identification based on the GA. Furthermore, it is possible to design an online controller of a SOFC stack based on this GA-RBF neural network identification model.

Key words: Solid oxide fuel cells (SOFCs), Radial basis function (RBF), Neural networks, Genetic algorithm (GA)
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INTRODUCTION

The solid oxide fuel cell (SOFC) has no liquid components and works in a complicated high-temperature (600~1000 °C) environment. Due to its high operation temperature, the SOFC has many advantages, such as high energy conversion efficiency, flexibility of usable fuel type, and high temperature exhaust gas, which make the SOFC a promising candidate for future energy conversion systems.

Analysis of the dynamics of SOFC systems reveals that the SOFC system is a nonlinear multi-input and multi-output system, which is hard to model by using the traditional methodologies. During the last several decades, various mathematical models have been established in the research on the internal mechanisms, ranging from a zero dimensional model to a three dimensional models (Lunghi and Ubertini, 2001; Bove *et al*., 2005; Nehter, 2006; Recknagle *et al*., 2003). Although these models are very useful for fuel cell design and performance analysis, they have some limits. Most of the models are based on mass, energy and momentum conservation laws, so their expressions are too complicated to be suitable for engineering applications.

Motivated by this need, some researchers have attempted to establish novel fuel cell models by statistical data-driven approach. Arriagada *et al*.(2002) utilized artificial neural network (ANN) methodology to derive a SOFC model. Highly efficient as the model is, however, its practical design suffered from some drawbacks such as the existence of local minima and over-fitting, choice of the number of hidden units, etc. A least squares support vector machine (LS-SVM) was used to build the model of a SOFC stack by Huo *et al*.(2006). LS-SVM is a modification of SVM and has many advantages. However this paper only considered the fuel utilization, which had effect on the cell voltage, and did not think about the other factors.

In this work, a radial basis function (RBF) neural network based on a genetic algorithm (GA) is employed to establish a black-box model for the SOFC. The RBF neural network is a feed-forward neural network with one hidden layer and can uniformly approximate any continuous function to a prespecified accuracy (Warwick, 1996). However, a key problem using the RBF neural network approach is how to choose the optimum initial values of the following three parameters: the output weights, and centers and widths of the hidden unit. If they are not appropriately chosen, the RBF neural network may degrade the validity and accuracy of modelling. To assure the optimal performance of the RBF neural network approach for SOFC modelling, we consider applying a GA to optimize the RBF neural network parameters in this study.

GA is a kind of self-adaptive global searching optimization algorithm based on the mechanics of natural selection and natural genetics (Goldberg, 1989). Different from conventional optimization algorithms, GAs are based on population, in which each individual is evolved parallelly, and the ultimate result is included in the last population. According to the characteristic of the least squares algorithms, algorithms, such as Levenberg-Marquardt and Gauss-Newton, were developed. But these methods have universal shortcomings such as slow convergence, sensitivity of initial value and lack of local optimization. GA is an effective method to overcome the above problems since its principle is the calculation of the coding rather than the parameters (Balland *et al.*, 2000). Instead of derivative, the object function is related to fitness value. Because of their relative simplicity and robustness, GA is becoming more popular.

DESCRIPTION AND ANALYSIS OF SOFC STACK

A SOFC is a device which converts chemical energy of a fuel directly into electrical energy. The basic components of the SOFC are anode, cathode and two ceramic electrodes. In the fuel cell, fuel is supplied to the anode and air is supplied to the cathode. At the cathode electrolyte interface, oxygen molecules accept electrons coming from the external circuit to form oxide ions. The electrolyte layer allows only oxide ions to pass through and at the anode-electrolyte interface, hydrogen molecules present in the fuel react with oxide ions to form steam and electrons are released. These electrons pass through the external circuit and reach the cathode-electrolyte layer, thus the circuit is closed. Eqs.(1)~(5) give the electrochemical reactions (Hall and Colclaser, 1999):

$$\text{Anode side:}\quad H_2 + O^{2-} \rightarrow H_2O + 2e^-, \tag{1}$$

$$CO + O^{2-} \rightarrow CO_2 + 2e^-; \tag{2}$$

$$\text{Cathode side:}\quad \frac{1}{2} O_2 + 2e^- \rightarrow O^{2-}; \tag{3}$$

Balance reactions:

$$(1)+(3):\quad H_2 + \frac{1}{2} O_2 \rightarrow H_2O; \tag{4}$$

$$(2)+(3):\quad CO + \frac{1}{2} O_2 \rightarrow CO_2. \tag{5}$$

A single cell produces an open-circuit voltage of approximately 1 V, so fuel cells have to be connected together in a series arrangement to form a stack.

For a given SOFC stack, the relation between terminal voltage U and current density I is influenced by many operating parameters, such as the operation pressure, temperature, air flow rate, hydrogen flow rate, etc. However, due to the great number of operating variables, a complete experimental database of SOFC under different operating conditions is difficult to obtain and no data are available in the literature yet (Costamagna *et al.*, 2001). Up to now, almost no models have ever been able to accommodate all these operating variables. Our GA-RBF model is no exception. In our experiment, current density I, which is decided by the uncontrollable load variables and cell operation pressure P are taken as variables.

In general, a wide class of nonlinear systems can be described by nonlinear autoregressive model with exogenous inputs (NARX) (Sjoberg *et al.*, 1995). So in this paper the SOFC nonlinear system with two inputs and one output can be described as follows:

$$U(k+1)=f[U(k),U(k-1),\ldots,U(k-n),I(k),I(k-1),\ldots,I(k-m),P(k)]. \tag{6}$$

Supposing there is a series of inputs $I(k)$, $I(k-1),\ldots,I(k-m),P(k)$ and outputs $U(k),U(k-1),\ldots,U(k-n)$. The aim of our study is thus to find a GA-RBF model that can approximate Eq.(6).

GA-RBF NEURAL NETWORK FOR NONLINEAR SYSTEM MODELLING

RBF theories

A RBF neural network has an input layer, a nonlinear hidden layer and a linear output layer. The nodes within each layer are fully connected to the previous layer nodes. The input variables are each assigned to nodes in the input layer and connected directly to the hidden layer without weights. The hidden layer nodes are RBF units. The nodes calculate the Euclidean distances between the centers and the network input vector, and pass the results through a nonlinear function (Ai-Amoudi and Zhang, 2000). The output layer nodes are weighted linear combinations of the RBF in hidden layer. The structure of a RBF neural network with M inputs, L outputs and q hidden nodes is given in Fig.1.

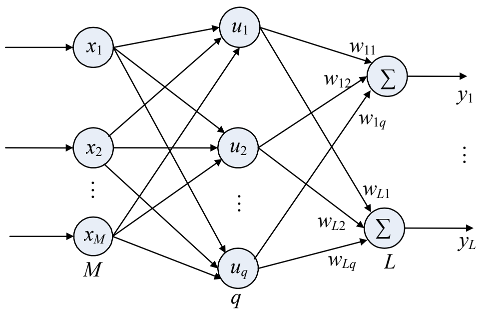

Fig.1 The structure of RBF neural networks

In Fig.1, input $\boldsymbol{x}=(x_1,x_2,\ldots,x_M)^{\mathrm{T}}$, output $\boldsymbol{y}=(y_1,y_1,\ldots,y_L)^{\mathrm{T}}$, and w_{ki} is the neural network weight. u_i is a nonlinear function and here it is chosen as a Gaussian activation function

$$u_i=\exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{c}_i)^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{c}_i)}{2\sigma_i^2}\right],\quad i=1,2,\ldots,q,\qquad (7)$$

where $\boldsymbol{c}_i=(c_{i1},c_{i2},\ldots,c_{iM})^{\mathrm{T}}$ is the center of the ith RBF hidden unit, and σ_i is the width of the ith RBF hidden unit. Then the ith RBF network output can be represented as a linearly weighted sum of q basis functions

$$y_k=\sum_{i=1}^{q}w_{ki}u_i,\qquad k=1, 2,\ldots,L,\qquad (8)$$

where w_{ki} are the weights. With the structure described above, the transformation from the input layer to the hidden layer is nonlinear, due to the use of Gaussian functions for RBF, and the connection of the hidden layer to the output layer is linear.

Design of GA-RBF

When we program to realize the RBF algorithm, how to choose the optimum initial values of the following three parameters in Eqs.(7) and (8): the output weight w_{ki}, the centers $\boldsymbol{c}_i$ and widths σ_i, is very important. If they are not appropriately chosen, the RBF neural network may degrade the validity and accuracy of modelling. So a GA is used to optimize the RBF neural network parameters.

GA is an interactive procedure that maintains a population of strings which constitute the set of candidate solutions to the specific problem (Gao *et al.*, 2000). During each generation, the strings in the current population are rated for their effectiveness as solutions. On the basis of these evaluations, a new population of candidate solutions is formed by using genetic operators. There are four major steps required to use GA to solve a problem and the main operations are as follows.

1. Coding structure

Coding aims to build the relationship between the problem and the individual in genetic algorithms. The population contains a number of individuals. Each individual represents a variable or a part of the problem which is needed to be optimized. In this paper, the parameters of RBF neural networks are optimized by GA. So these genes represent the output weights, centers and widths of the Gaussian function.

2. Fitness function evaluation

All individuals of one generation are evaluated by a fitness function. When using a genetic algorithm to solve a problem, the problem is represented by a string, and an evaluation function is defined. The evaluation function uses the value of the sting as a parameter to evaluate the results of the problem. Each string is evaluated through the evaluation function and the new generation is formed by using the specific genetic operators. Here a RBF neural network is used to model a SOFC stack. In order to get higher precision, the fitness function f is defined as

$$f=J^{-1}=\left(50\sum_{i=1}^{N}\left|e(i)\right|\right)^{-1},\qquad (9)$$

where J is the goal function and $e(i)$ is the error between the experimental output and the model output.

3. Genetic operations

Generally the genetic operators are selection, crossover and mutation. These genetic operations have key effects on the performances of the genetic algorithm. In the selection operation, an individual is probabilistically selected from the population on the basis of its fitness and the selected individual is then copied without any change into the next generation of the population. Crossover starts with two parents independently selected probabilistically from the population on the basis of their fitness. The mutation operation is done to escape the local minima in the search space of the artificial genetic approach. A position of a random individual is chosen at random and the individual is replaced by another value, for example, a "0" and a "1" in binary representation. The total number of bits selected to mutate is settled by the mutation rate.

4. The terminate criterion

There are usually two criterions for terminating a run. The first criterion is deciding the maximum generation previously; the second is that the process continues until the fitness function has no change. Here we choose the first criterion and decide on the maximum generation.

MODELLING SOFC BASED ON GA-RBF

Training process of GA-RBF

In our study, a model (Calise *et al.*, 2006) is used to generate the data required for the training of the GA-RBF model. Here two groups of current density and cell voltage data at 3 bar and 9 bar are chosen as training data, and each group has 701 pairs of data. Main operational parameters of SOFC are varied, such as operation pressure (0~15 bar), stack current density (0~700 mA/cm^2). In most cases, training data should be scaled. In this paper, all the data, including cell voltage, current density and operation pressure, are scaled to [0,1] by Eq.(10):

$$x' = (x_i - x_{\min})/(x_{\max} - x_{\min}). \tag{10}$$

The structure of the RBF neural network is chosen 2-3-1, i.e. let the RBF neural network consist of input layer with 2 nodes, 1 hidden layer with 3 nodes and output layer with 1 node. The momentum factor is chosen as 0.6 and the learning rate is chosen as 0.53.

The parameters of the RBF neural network are trained by the genetic algorithm. These genes represent the weights, the center and width of the Gaussian function and the representation of an individual is

$$\boldsymbol{p}=[b_1\ b_2\ b_3\ c_{11}\ c_{12}\ c_{13}\ c_{21}\ c_{22}\ c_{23}\ w_1\ w_2\ w_3], \tag{11}$$

here each individual consists of 12 10-bit numbers. They are concatenation of the 3 connection weights, 6 centers and 3 widths of the hidden unit of the RBF neural network. We use Roulette wheel selection and take the control parameters of genetic algorithm as the population size 30, crossover probability p_c 0.8, mutation probability p_m 0.003−[1:1:*size*]×0.003/*size*. After 100 times genetic manipulations, the optimized parameters are: The optimized widths b_1, b_2, b_3 are 1.9880, 1.5146, 2.8724; the centers of the Gaussian function c_{11}, c_{12}, c_{13}, c_{21}, c_{22}, c_{23} are 0.3724, −0.8416, −0.5073, −1.7918, 1.6276, −2.7889, and the optimized output weights w_1, w_2, w_3 are −0.4174, 0.8397, 0.8690, respectively. The optimal value J in Eq.(9) is 121.3089.

Predicting with the GA-RBF model

After training, a GA-RBF model is obtained which can be used to predict new input data. In our study, the testing data are also chosen from the above-mentioned model (Calise *et al.*, 2006). The cell voltage at 6 bar and 12 bar with the current density in the range from 0 to 700 mA/cm^2 is predicted. And a comparison between the predicted data and the experimental data is made to evaluate the model's prediction precision (Fig.2). At the same time, a LS-SVM model is also used to predict the stack voltage at 6 bar and 12 bar. Via the LS-SVM toolbox (Chang and Lin, 2001), the predicted result is shown in Fig.3. Comparing Fig.2 with Fig.3, we can see clearly that the precision is greatly improved. It indicates that GA-RBF is a powerful tool for modelling SOFC and our GA-RBF model presented in this paper is accurate and valid.

CONCLUSION

To facilitate valid control strategy design, an offline modelling study of a SOFC stack using a GA-

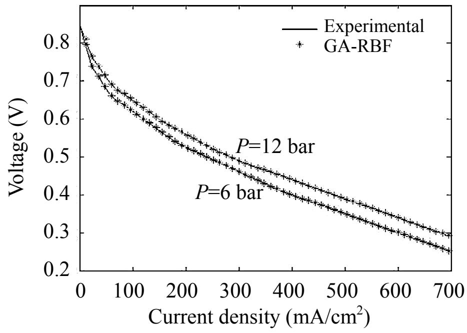

Fig.2 Voltage-current density characteristics: predicted by GA-RBF model and experimental *P*=6 bar and *P*=12 bar

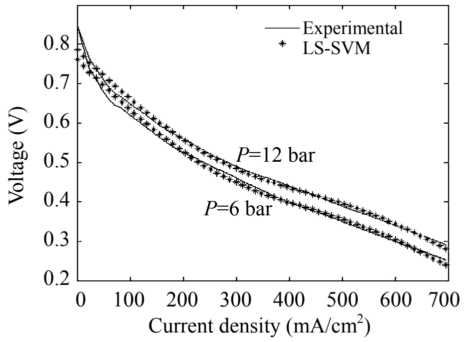

Fig.3 Voltage-current density characteristics: predicted by LS-SVM model and experimental *P*=6 bar and *P*=12 bar

RBF neural network is reported in this paper. It is shown that the GA-RBF model is more attractive and more competitive than other modelling solutions in that it avoids using complicated differential equations to describe the stack, and the input-output characteristics can be obtained rapidly by GA-RBF estimation. Besides, compared with the LS-SVM approach, the simulation results show that the GA-RBF approach yields higher prediction accuracy. Hence it is feasible to establish the model of the SOFC by using GA-RBF.

Among all the operating parameters that have an effect on the SOFC performance, only current density and operation pressure are included in our model. In the future we should incorporate any other operating parameters into the GA-RBF model, and based on this GA-RBF model, some control scheme studies such as predictive control and robust control can be developed.

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