A Hybrid Experimental Model of a Solid Oxide Fuel Cell Stack

A multivariable hybrid experimental model of a solid oxide fuel cell stack is developed in this paper. The model consists of an improved radial basis function (RBF) neural network model and a pressure-incremental model. The improved RBF model is built to predict the stack voltage with different temperatures and current density. Likewise, the pressure-incremental model is constructed to predict the stack voltage under various hydrogen, oxygen, and water partial pressures. We combine the two models together and make a powerful hybrid multivariable model that can predict the voltage under any current density, temperature, hydrogen, oxygen, and water partial pressure. The validity and accuracy of modeling are tested by simulations, and the simulation results show that it is feasible to build the hybrid multivariable experimental model. [DOI: 10.1115/1.2971125]

Keywords: solid oxide fuel cell (SOFC), hybrid model, radial basis function (RBF), genetic algorithm (GA), pressure-incremental model

1 Introduction

Unlike other fuel cells, solid oxide fuel cell (SOFC) is entirely a solid state with 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.

According to analysis of the dynamics of SOFC systems, it is known that the SOFC system is a nonlinear multi-input and multioutput system, which is hard to model. 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 model [1–4]. Although these models are very useful for fuel cell design and performance analysis, they have some limits. Most of these models emphasized the detailed description of cell internal processes. What matters most to SOFC users are not its relevant internal details but its performances under different operating conditions.

To meet the demands, some researchers have attempted to establish novel fuel cell models by statistical data-driven approach. Arriagada et al. [5] utilized artificial neural network (ANN) methodology to derive a SOFC model. An adaptive network-based fuzzy inference system (ANFIS) identification model for a SOFC stack has been presented in Ref. [6]. Dynamic modeling of a SOFC system based on a T-S fuzzy model is proposed in Ref. [7]. Although the temperature, hydrogen, oxygen, and water partial pressures are the most important controllable variables for a SOFC system, the proposed models cannot deal with all of them simultaneously. One important reason is that a complete experimental database of SOFC under various operating conditions is difficult to obtain, and no data are available in the open literature yet [8].

To solve this problem, a multiple variable hybrid model is proposed in this paper. This model consists of two parts: One is an improved radial basis function (RBF) neural network model that concerns current density and temperature [9]. The RBF neural network is a feedforward neural network with one hidden layer, which can uniformly approximate any continuous function to a prespecified accuracy [10]. To assure the optimal performance of the RBF neural network, genetic algorithm (GA) is used to optimize the RBF neural network parameters. The other part of the hybrid model is a pressure-incremental model, which is developed to expand our proposed GA-RBF model to other pressures. Therefore, in this paper only limited numbers of empirical data are needed to build the hybrid experimental model, which can deal with current density, temperature, hydrogen, oxygen, and water partial pressures simultaneously.

2 Theoretical Analysis

For a given SOFC stack, the relation between terminal voltage $U$ and current density $I$ is influenced by many operating parameters, such as cell temperature, oxygen pressure, hydrogen pressure, water pressure, etc. In general, a wide class of nonlinear systems can be described by nonlinear autoregressive model with exogenous inputs (NARX) [11]. Therefore, in this paper the SOFC nonlinear system can be described as follows:

$$U = f(I,T,P_{H_2},P_{O_2},P_{H_2O} \cdots)$$

Due to its high dimensionality, it is hard to model Eq. (1) with traditional ways. Therefore, Eq. (1) is separated into two parts.

$$U = U^0(I,T) + U_{AP}(\Delta P_{H_2}, \Delta P_{O_2}, \Delta P_{H_2O})$$

The first part $U^0$ denotes a GA-RBF model, which predicts voltage at different current density and temperature under a constant hydrogen pressure $P_{H_2}^0$, a constant oxygen pressure $P_{O_2}^0$, and a constant water pressure $P_{H_2O}^0$. These constant pressures are referred to as the reference pressures. The second part $U_{AP}$ denotes a pressure-incremental model, which predicts voltage increment caused by oxygen pressure increment $\Delta P_{O_2}$, hydrogen pressure increment $\Delta P_{H_2}$, and water pressure increment $\Delta P_{H_2O}$. The structure of the proposed hybrid experimental model is shown in Fig. 1.

3 Hybrid Model

3.1 GA-RBF Model. Suppose the operating pressure of hydrogen, oxygen, and water of SOFC is kept constant in the GA-RBF model. The relation between terminal voltage $U$ and current density $I$ is mainly influenced by the temperature $T$. The following NARMAX model is used to describe the system

$$y(k) = f[y(k-1), y(k-2), \ldots, y(k-n_y), u(k-1), u(k-2), \ldots, u(k-n_u)]$$

where $y$ is the SOFC terminal voltage, $u$ is the temperature and
current density, $n_e$ and $n_a$ are the lags of the output and input, respectively, and $f(\cdot)$ is a nonlinear function. In this section, we adopt a GA-RBF neural network to identify the nonlinear function $f(\cdot)$. The structure of the RBF neural network is shown in Fig. 2.

The output of hidden layer is

$$u_i = \exp \left[ -\frac{(x - c_i)^T(x - c_i)}{2\sigma_i^2} \right] \quad (i = 1, 2, \ldots, q) \quad (4)$$

where $x = (I, T)^T$, $c_i = (c_{i1}, c_{i2})^T$ is the center of the $i$th RBF hidden unit, and $\sigma_i$ is the width of the $i$th RBF hidden unit.

The output is

$$y_R = \sum_{i=1}^{q} w_i u_i \quad (5)$$

where $y_R$ is the output voltage calculated from neural network, $y$ the voltage target value, and $M$ the number of training data. A gradient descent algorithm is adopted to minimize $J$. Also, the genetic algorithm is used to obtain the optimum initial values of the following three parameters: the output weight $w_i$, the centers $c_i$, and widths $\sigma_i$.

In order to make the model incorporate hydrogen, oxygen, and water partial pressures besides the current density and temperature, a huge amount of training data would be needed. Therefore, a pressure-incremental model is developed to expand our proposed GA-RBF model to other pressures.

3.2 Pressure-Incremental Model. Applying Nernst’s equation and Ohm’s law (taking into account Ohmic, concentration, and activation losses), the stack output voltage is represented as follows:

$$U = E - \eta_{\text{Ohmic}} - \eta_{\text{conc}} - \eta_{\text{act}} \quad (7)$$

Where the open circuit voltage $E$ is expressed as

$$E = N \left( E^* + \frac{RT}{2F} \ln \frac{P_{H_2}P_{O_2}^{1/2}}{P_{H_2O}} \right) \quad (8)$$

where $E^*$ is the standard cell potential, $N$ is the number of the cells (384), $F$ Faraday’s constant (96,485 c/mol), $R$ is the gas constant (8.314 J/mol K), $T$ is the cell temperature (K), $P_{H_2}$ is the partial pressure of hydrogen (atm), $P_{O_2}$ is the partial pressure of oxygen (atm), and $P_{H_2O}$ is the partial pressure of water (atm). $E^*$ exhibits a linear relationship with cell temperature and can be approximated from the experimental data provided in Ref. [12].

$$E^* = 1.2586 - 0.000252T \quad (9)$$

Hence, the open circuit voltage $E$ can also be written as

$$E = 483.40224 - 0.09677T + 0.01654T \ln P_{H_2} + 0.5 \ln P_{O_2} - \ln P_{H_2O} \quad (10)$$

Ohmic polarization occurs because of resistance to the flow of ions through different components of cell materials. The loss can be expressed as:

$$\eta_{\text{Ohmic}} = IR_{\text{Ohmic}} \quad (11)$$

where $R_{\text{Ohmic}}$ is the cell resistance, which is a function of cell electrode temperature and can be expressed by the second-order Steinhart-Hart equation.

$$R_{\text{Ohmic}} = \lambda_1 \exp \left[ \lambda_2 \left( \frac{1}{T} - \frac{1}{T_0} \right) \right] \quad (12)$$

Where $T$ is the stack temperature, and $\lambda_1$, and $\lambda_2$ are constant coefficients. The Ohmic loss is independent of the pressure, which has no influence on our pressure-incremental model and could be neglected.

The concentration and activation loss equation can be calculated by the following equations:

$$\eta_{\text{conc}} = \lambda_3 \ln \left( 1 - \frac{I}{I_L} \right) \quad (13)$$

$$\eta_{\text{act}} = \lambda_4 + \lambda_5 \log I \quad (14)$$

where $\lambda_3$, $\lambda_4$, and $\lambda_5$ are the coefficients, and $I_L$ is the limiting current. The loss is independent of the pressure, which has no influence on our pressure-incremental model and could be neglected.

Let $P_{H_2}^0$, $P_{O_2}^0$, and $P_{H_2O}^0$ stand for the given reference partial pressures of hydrogen, oxygen, and water, respectively, under which the GA-RBF model predicts the SOFC voltage at different current densities and temperatures, by Sec. 3.1. The hydrogen, oxygen, and water pressure increments are defined as the proportional form:

$$P_{H_2} = k_{H_2} P_{H_2}^0, \quad P_{O_2} = k_{O_2} P_{O_2}^0, \quad P_{H_2O} = k_{H_2O} P_{H_2O}^0 \quad (15)$$

With the substitution of Eqs. (10)–(15) into Eq. (7), the SOFC voltage can be rewritten as:

$$U = U^0 + U_{\Delta P} \quad (16)$$
where $U$ pressure-incremental model.

In order to reduce the numbers of the parameters and improve the identification of the GA-RBF model and the proposed hybrid experimental model, the root mean square error (RMSE) is employed here to evaluate modeling results, which is calculated by

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{k=1}^{N} (y(k) - \hat{y}(k))^2}$$

where $N$ is the number of sample data from the dynamic physical model of SOFC, $y(k)$ is the predictive output, and $\hat{y}(k)$ is the output of the dynamic physical model.

First, for the purpose of the GA-RBF model identification, the dynamic physical model is uniformly random input signals including the temperature (600–1000°C) and the current density (0–800 mA/cm²). Air, hydrogen, and water pressures are all regulated to 3 atm. To obtain the dynamic physical model output voltage values at integer time points, the fourth-order Runge–Kutta method is used to find the numerical solution in the simulation via the MATLAB. A set of 3000 data is collected from the simulation. The first 1000 data are used for the identification of the GA-RBF model, while the remaining 2000 data are used for validation purposes.

In order to reduce the numbers of the parameters and improve the speed of program debug, the hidden layer of the RBF neural network has chosen 3 nodes. After many trials, a population size of 60, a crossover probability of 0.35, and a mutation probability of 0.001 are used. The optimized initial values of the parameters mentioned above The Sec. 3.1 are shown in Table 1.

After the optimized initial values of the three parameters are obtained, we utilize the gradient descent learning algorithms to adjust them. After training, a GA-RBF model is obtained, which can be used to predict a new input date. Under various temperatures and current densities, the voltage identification model is shown in Fig. 3. The RMSE of the output voltage obtained is 0.6285. The result shows that the GA-RBF neural network can approximate the behavior of the physical SOFC model with good accuracy.

The GA-RBF model has been built to predict the voltages when oxygen pressure, hydrogen pressure, and water pressure are all 3 bars with temperatures from 800°C to 1000°C. Using this prediction as reference data, the pressure-incremental model can be made to take the prediction at other pressures. Now in order to validate the proposed hybrid experimental model, the dynamic model developed by the Ref. [13] is uniformly random input signals including the oxygen pressure, hydrogen pressure, water pressure (1–10 atm), temperature (600–1000°C), and current density (0–800 mA/cm²). The fourth-order Runge–Kutta method is also used to find the numerical solution to the dynamic physics model in the simulation. Experimental data are obtained with temperature of 750°C, current density of 2 mA/cm², and various pressures, which are listed in Table 2. The first group is used as reference data for our predictions, and the other three groups to verify our predictions. Based on the reference data, Eq. (18) can help predict voltages under other pressures. From Table 2, we can see that the obtained hybrid experimental model can approximate the physical SOFC stack model with good accuracy.

### Table 1 The optimized initial values of widths, centers, and output weights

<table>
<thead>
<tr>
<th>$b_1$</th>
<th>$b_2$</th>
<th>$b_3$</th>
<th>$c_{11}$</th>
<th>$c_{12}$</th>
<th>$c_{13}$</th>
<th>$c_{21}$</th>
<th>$c_{22}$</th>
<th>$c_{23}$</th>
<th>$w_1$</th>
<th>$w_2$</th>
<th>$w_3$</th>
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<tr>
<td>1.2346</td>
<td>1.3784</td>
<td>0.5732</td>
<td>-0.5897</td>
<td>-0.4352</td>
<td>0.3459</td>
<td>1.2385</td>
<td>-1.0376</td>
<td>1.3986</td>
<td>0.4986</td>
<td>0.8760</td>
<td>0.6706</td>
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</table>

### Table 2 Errors between actual voltage and hybrid experimental model

<table>
<thead>
<tr>
<th>No.</th>
<th>$P_{O_2}/k_O_2$ (atm)</th>
<th>$P_{H_2}/k_{H_2}$ (atm)</th>
<th>$P_{H_2O}/k_{H_2O}$ (atm)</th>
<th>Actual voltage (V)</th>
<th>Predicted voltage (V)</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1/−</td>
<td>1/−</td>
<td>1/−</td>
<td>370.206</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>2</td>
<td>1.5/1.5</td>
<td>2/2</td>
<td>1.5/1.5</td>
<td>374.6358</td>
<td>371.8024</td>
<td>0.7563</td>
</tr>
<tr>
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<td>2/2</td>
<td>1.5/1.5</td>
<td>1.5/1.5</td>
<td>373.9476</td>
<td>371.4548</td>
<td>0.6666</td>
</tr>
<tr>
<td>4</td>
<td>1.5/1.5</td>
<td>1.5/1.5</td>
<td>1.5/1.5</td>
<td>372.7865</td>
<td>371.2398</td>
<td>0.4149</td>
</tr>
</tbody>
</table>

Fig. 3 Voltage-current characteristics predicted by the GA-RBF model and experimental data at T=800°C, 900°C, and 1000°C
water partial pressures, is reported in this paper. The model consists of two parts. One is the GA-RBF model that concerns current density and temperature. The other one is the pressure-incremental model that concerns hydrogen, oxygen, and water partial pressures. The simulation results show that the hybrid approach yields higher prediction accuracy. Hence, it is feasible to establish the model of SOFC by using the hybrid model.

References


