Modeling and Simulation of Solid Oxide Fuel Cell Based On Neural Network

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Abstract. In order to study the effects of hydrogen input molar flow, oxygen input molar flow, water vapor input molar flow and real-time temperature on the output voltage of solid oxide fuel cell (SOFC), this paper proposes a method to model SOFC using a BP neural network optimized by immunogenetic algorithm (IA). MATLAB simulation results show that the SOFC model established in this paper can more accurately reflect the actual SOFC input and output characteristics. And the model has a high fit to the real data.

1. Introduction
Solid oxide fuel cell (SOFC) is a kind of all-solid battery that directly converts chemical energy in fuel gas and oxide gas into electrical energy and is characterized by nonlinearity, strong coupling, complex internal structure and susceptible to external influences. The analysis and modeling of the input and output characteristics of SOFC will be of great practical significance for SOFC power generation systems and will provide some guidance for the control of new energy battery [1].

A large number of literature studies on the main influencing factors of SOFC output performance show that the hydrogen input molar flow rate, oxygen input molar flow rate, water vapor input molar flow rate, and real-time temperature all have effect on the output characteristics of SOFC. In literature [2], a SOFC model with fuel flow, air flow, furnace temperature, and current to predict the voltage and temperature of the cell was established using BP neural network, achieving an average relative error of 0.2% between the predicted and measured results. In literature [3], Tang Shui established a three-dimensional model based on COMSOL Multi-Physice 5.3 simulation platform to numerically calculate and analyzed the effects of cell length, operating temperature, current density, and inlet air composition on the operating performance of the solid oxide fuel cell. In literature [4], Xiao Li used the reaction mechanism of SOFC to establish the SOFC model to obtain the input-output data, and then used the system identification toolbox in MATLAB to identify the SOFC mathematical model. A neural network model was developed in literature [5] for predicting the performance of solid oxide fuel cells, prediction of battery voltage and power using back propagation algorithm and comparison with physical nonlinear model results. The neural network structure based on Levenberg Marquardt back propagation algorithm got more suitable for modeling the characteristics of nonlinear solid oxide fuel cells. In literature [6], an artificial neural network was used to model the anode of a solid oxide battery and optimize the parameters of the SOFC using a genetic algorithm to achieve the maximum power output of the SOFC under different parameters. In literature [7] and [8], Wenhan Zhong and Chunming Song used data modeling approach to build a SOFC model with BP neural network. The error between the output voltage of the model and the desired voltage was in the range of -2% to 6%.
In literature [9], Dongyan Liu modeled the SOFC system with BP neural network and obtained the predicted value of temperature with an error of only 0.011% of the SOFC test system in the fuel cell research center of Huazhong University of Science and Technology, which improved the prediction accuracy of temperature in SOFC. In paper [10], Kang Xin established a kinetic model for methane water vapor reforming (MSR) reaction based on the working principle of SOFC. In paper [11], Wu Lihua optimized the parameters of RBF neural network by particle swarm algorithm and used it in the modeling of SOFC to solve the problem of inaccurate initial parameters, reduced the accuracy of the model.

In SOFC modeling, the model established by BP neural network has higher accuracy and smaller error. It can reflect the output performance of SOFC more accurately. In this paper, the establishment of SOFC mechanism model to get the simulation experimental data, using the immune genetic algorithm optimization of BP neural network to establish the SOFC model, in order to get a more accurate reflection of the actual work of SOFC model.

2. SOFC mechanism modeling

According to the SOFC electrochemical reaction equation, the output voltage of SOFC cell considering the concentration, activation, and ohmic loss is shown in equation (1).

\[
U_{\text{cell}} = E^0 + \frac{RT}{2F} \ln \left( \frac{P_{\text{H}_2} \cdot P_{\text{O}_2}^{0.5}}{P_{\text{H}_2\text{O}}} \right) - r_0 \exp \left[ \alpha \left( \frac{1}{T} - \frac{1}{T_0} \right) \right] I - (a + b \log I) - \frac{RT}{2F} \ln \left( 1 - \frac{1}{I_L} \right) \tag{1}
\]

Assume that the pressure in the gas flow path is constant and that the ratio of internal to external pressure is sufficient. According to the conservation of mass, the partial pressures of hydrogen, oxygen, and water vapor inside the SOFC is shown in equation (2).

\[
\begin{align*}
\frac{dP_{\text{H}_2}}{dt} &= \frac{T}{k_{\text{H}_2} \tau_{\text{H}_2} T_0} \left( n_{\text{in}}^{\text{H}_2} - k_{\text{H}_2} P_{\text{H}_2} - 2k_r I \right) \\
\frac{dP_{\text{O}_2}}{dt} &= \frac{T}{k_{\text{O}_2} \tau_{\text{H}_2} T_0} \left( n_{\text{in}}^{\text{O}_2} - k_{\text{O}_2} P_{\text{O}_2} - k_r I \right) \\
\frac{dP_{\text{H}_2\text{O}}}{dt} &= \frac{T}{k_{\text{H}_2\text{O}} \tau_{\text{H}_2} T_0} \left( n_{\text{in}}^{\text{H}_2\text{O}} - k_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}} + 2k_r I \right)
\end{align*}
\tag{2}
\]

The meaning of each symbol in equation (1) and (2) is shown in Table 1.

| Symbols | Meaning                  | Symbols | Meaning                |
|---------|--------------------------|---------|------------------------|
| P       | Ideal gas pressure       | R       | General Gas Constants  |
| E       | Electromotive force      | E^0     | Standard Battery Electric Potential |
| n^{in}  | Input molar flow of gas  | r_0     | Internal resistance to battery start temperature |
| T_0     | Starting Temperature     | I       | Battery Current        |
| b       | Tafel slope              | I_L     | Battery Limit Current  |
| T       | Battery reflection temperature | α       | Constant coefficient of the battery |
| F       | Faraday's Constant       | a       | Tafel's constant       |

According to equation (1) and equation (2), the SOFC simulation model is built in Simulink, as shown in Figure 1. It can be concluded that when the hydrogen input molar flow rate, oxygen input molar flow rate, water vapor input molar flow rate, real-time temperature and SOFC output voltage have a complex non-linear relationship. In particular, the relationship between the real-time temperature and the SOFC output voltage. On low current and low temperature, the SOFC output voltage is higher. On high current and high temperature the SOFC output voltage is also higher. Both
temperature-dependent activation and ohmic polarization losses decrease as the load current increases, while activation and ohmic polarization losses decrease as the temperature of SOFC increases.

3. SOFC BP neural network model establishment

The model based on the input-output characteristics of the SOFC is highly nonlinear. BP neural network is a multilayer feedforward neural network with implicit layers that can approximate arbitrary nonlinear mappings. Use BP neural network built SOFC model will be more suitable for control and facilitate in-depth analysis of the SOFC input and output characteristics.

In this paper, we study the effects of hydrogen input molar flow $n_{\text{H}_2}^\text{in}$, oxygen input molar flow $n_{\text{O}_2}^\text{in}$, water vapor input molar flow $n_{\text{H}_2\text{O}}^\text{in}$, and real-time temperature $T$ on the output voltage $U$ of the SOFC. Therefore, in the structural design of the BP neural network, the four input layer neurons are taken as $x_1 = n_{\text{H}_2}^\text{in}, x_2 = n_{\text{O}_2}^\text{in}, x_3 = n_{\text{H}_2\text{O}}^\text{in}, x_4 = T$. The output layer neuron is the output voltage $U$, while the implicit layer neuron needs to be constantly adjusted according to the actual simulation. According to the empirical formula:

$$m = \sqrt{n + l + a} \quad (3)$$

In the formula, $n$ is the number of input variables, $l$ is the number of output variables, and $a$ is an integer between 1 and 10. With experiments and comparisons, it is concluded that the higher the number of nodes in the hidden layer, the higher the accuracy, as well as the increase in simulation time. Since this thesis mainly considers the accuracy of SOFC model, the number of neurons in the hidden layer is taken as the maximum value 12. The three-layer BP neural network model with a structure of 4-12-1 is used to model the SOFC, and Figure 2 shows the neural network model.

The input $net_i$ of the implicit layer is:

$$net_i = \sum_{j=1}^{4} \omega_{ij}x_j \quad (4)$$

where $\omega_{ij}(i = 1 \ldots 12)$ is the weight between the input layer and the implied layer.

The output $o_i$ of the implicit layer is:

$$o_i = f(net_i - \theta_i) \quad (5)$$

where $f$ is the sigmoid excitation function and $\theta_i$ is the threshold of the implicit layer neuron $i$.

The total input $net_k$ for the $k$th neuron of the output layer is:

$$net_k = \sum_{i=1}^{12} \omega_{ki}o_i \quad (6)$$

where $\omega_{ki}(i = 1 \ldots 12, k = 1)$ is the connection weight between neuron $i$ in the implicit layer and neuron $k$ in the output layer.

Then the mathematical expression for the BP neural network model of SOFC can be expressed as equation (7).

$$y = f(net_k - \theta_j) \quad (7)$$
where $y = U$ is the output value of the BP neural network and $\theta_j$ is the threshold value of the output layer neuron $j$.

Using mean-square error (MSE) as the optimization target. The mean square error of the output layer can be calculated in equation (8).

$$E = \frac{1}{2} (\hat{y} - y)^2$$

$\hat{y}$ is the output voltage of the mechanistic model (i.e., the actual voltage), and $y$ is the output voltage of the neural network (i.e., the predicted voltage).

The correction amount of the weights $\omega$ is:

$$\Delta \omega = -\eta \frac{\partial E}{\partial \omega}$$

where $\eta$ is the learning rate parameter: $\eta = \text{lrb} \times \text{lrd} \times \text{gs} \times \text{lrs}$, $\text{lrb}$ is the initial value of the learning rate, $\text{lrd}$ is the learning rate decay rate (between 0 and 1), $\text{gs}$ is the number of iterations, and $\text{lrs}$ is the momentum factor (the frequency with which the learning rate is updated, i.e., how many iterations to update the learning rate).

According to equation (1) and equation (2), build the SOFC mechanism model in Simulink and set the parameters in conjunction with the actual working condition of the SOFC. 500 sets of SOFC input and output data were collected, of which 400 sets were randomly selected as BP neural network training data, and the remaining 100 sets were used as BP SOFC output voltage prediction data. Figure 3 shows the error curve of the BP SOFC model output voltage, the results show that the output voltage error of the SOFC model built with BP neural network is between -0.1v and 0.1v.

4. Improved neural network modelling of SOFC

4.1. GA - BP neural network based model for SOFC

Although BP neural network can reflect the SOFC input-output characteristics, it is easy to fall into local minima and has relatively large error. A genetic algorithm is added to optimize the weights and thresholds of the BP neural network, it can avoid the BP network from falling into local minima and speed up the convergence rate. Using the elimination mechanism of the genetic algorithm, the trained population becomes more optimal. The flow of genetic algorithm is shown in Figure 4.
The output voltage versus actual voltage curve obtained using the genetic algorithm is shown in Figure 5, and the voltage error plot is shown in Figure 6. From Figures 5 and 6, we can see that the output voltage range of the SOFC model built with GA-BP neural network is between 0.843v and 0.846v. And the error between the actual voltage (output voltage of the mechanism model) and the predicted voltage (output voltage of the neural network model) is between -0.008v and 0.008v. Comparing Figure 3 with Figure 6, the output voltage error of the GA-BP SOFC model is two orders of magnitude lower than that of the BP SOFC model.

4.2. IA - BP neural network based model for SOFC

Since genetic algorithms are prone to local solutions, this paper adopts immunogenetic algorithm to improve traditional genetic algorithm. Immunogenetic algorithm retains random global parallel search feature of genetic algorithm, improves local and global search capability, and avoids premature convergence as much as possible. So that the final result tends to be globally optimal. The mean square error in BP neural network is used in the optimization of BP neural network with immunogenetic algorithm. The square of the difference between the network output and the target value is then averaged as the optimization objective. The flowchart of the immunogenetic algorithm (IA) is shown in Figure 7.

The output voltage curves and error curves of the BP neural network prediction optimized by the immunogenetic algorithm are shown in Figures 8 and 9.
From Figure 8 and 9, it can be seen that the output voltage of the SOFC model predicted by the IA-BP neural network does not differ from the ideal single-cell voltage of 0.85v by more than 0.003v, which is smaller and more accurate than the output voltage of the SOFC predicted by GA-BP.

Table 2. BP, GA-BP, IA-BP SOFC output voltage error range.

| Neural Networks | Minimum Error | Maximum Error |
|-----------------|---------------|---------------|
| BP              | -0.1v         | 0.1v          |
| GA-BP           | -0.007v       | -0.004v       |
| IA-BP           | -0.003v       | -0.003v       |

As can be seen from Table 2, comparing the results of modeling the SOFC by BP, GA-BP, and IA-BP respectively, it can be seen that the output voltage of the immunogenetic algorithm optimized BP neural network SOFC model is very close to the ideal output voltage of 0.85v for a single cell, and the error is close to 0.003v. The output voltage error of IA-BP SOFC is smaller than that of BP SOFC and GA-BP SOFC model.

5. Conclusion
In this paper, according to SOFC mechanism modeling, 500 experimental data were collected. Among them, 400 sets of data are used as training data, and the remaining 100 sets of data are used as prediction data. The molar flow of hydrogen, the molar flow of oxygen, the molar flow of water vapor and the temperature are taken as the input and the voltage is taken as the output. The prediction models of SOFC output voltage were developed using BP, GA-BP and IA-BP networks, respectively. The comparison shows that the output voltage error of the SOFC model built by the BP neural network optimized by immunogenetic algorithm is as low as 0.003v, which has a good accuracy. It lays the foundation for the future design of controller, battery stack and SOFC power generation system.

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