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Research and comparison of modeling methods of solid oxide fuel cell

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Abstract

Solid oxide fuel cell (SOFC) is a nonlinear, strongly coupled, large hysteresis system. In this paper, SOFC mechanism model is established according to the laws of mass conservation, energy conservation and electrochemical conservation. SOFC steady-state and transient characteristics are studied to understand the internal change mechanism. In order to predict SOFC performance, a BP neural network model optimized by genetic algorithm was established, and the neural network model training data were generated by the mechanism model. The results show that the BP neural network optimized by genetic algorithm is superior to the unoptimized BP neural network, and the BP neural network optimized by genetic algorithm is used to predict the performance of SOFC at different temperatures. The results show that the neural network can fit and predict the performance of SOFC well.

Keywords

SOFC; genetic algorithm; BP neural network; lumped model.

1. Introduction

In recent years, energy resources have become increasingly scarce, and the environmental pollution problems caused by fossil energy are numerous, which makes people have to carry out energy transformation and focus on clean and renewable energy. Fuel cell has become the focus of attention due to its superior performance. Solid oxide fuel cell (SOFC), with its advantages of zero emissions, low pollution, fuel diversity and high efficiency, become the most popular type of battery. Therefore, SOFC systems have been applied to areas such as military, traffic and housing [1].

Because the actual operating environment of SOFC is complex, it is difficult to obtain the internal operating state of the cell, resulting in slow research progress. Scholars study the internal mechanism and performance of SOFC through modeling and simulation. In reference [2], the three-dimensional model of SOFC is studied by using fluid simulation software FLUENT, and the SOFC performance under different inlet flow rate, different pressure and different inlet temperature is obtained. The concentration distribution of each component in the stack is analyzed to provide a basis for the design of the SOFC stack. In reference [3], COMSOL is used to study the internal temperature and temperature gradient distribution of single channel SOFC. In reference [4], the two-dimensional SOFC model is studied, and the effects of different gas parameters and cell structure parameters on the internal electrochemical reaction and output power of SOFC are discussed. In reference [5], a control model of SOFC system is proposed, which uses machine learning algorithm to find the maximum output power of SOFC at different operating temperatures. Lyapunov theory is used to study the local stability of the equilibrium point to help build the controller of SOFC system.

Lumped model and the neural network model can describe the dynamic characteristics of SOFC. Lumped model was established by the mathematic expression of the complex model, the

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equivalent of a white box model, through the lumped model can understand operation principle of SOFC. The neural network model was established through the study of the fitting of experimental data of a black box model, it can only describe the running characteristics of the SOFC, and unable to know the internal principle. The cost of verifying the neural network model through actual experimental data is relatively high, so the lumped model can be used to provide data for the neural network model to verify its applicability.

At first, this paper established a SOFC lumped model, by adjusting the lumped parameter model to make it with the actual test data to achieve the best fitting effect. Next, set up a BP neural network model and genetic algorithm to optimize the BP neural network model, the training of the neural network model used to verify the fitting and forecast data are produced by lumped model under different operating conditions. By comparing the BP neural network model and the BP neural network model optimized by genetic algorithm, the neural network model with good performance was selected to predict the performance of SOFC at different operating points. Finally, the model with good performance was used to fit the actual test data, and the fitting performance of the lumped model and the neural network model was compared.

The rest of this paper is described as follows: 1) establish SOFC lumped model; 2) The steady-state and transient characteristics of SOFC are analyzed based on lumped model; 3) BP neural network optimized by genetic algorithm is used to predict and analyze the performance of SOFC; 4) Conclusion.

2. Mathematical Model

SOFC is composed of anode, cathode and solid electrolyte. SOFC operation principle is shown in Fig.1, the role of oxygen in the cathode catalyst under electron into oxygen ions, oxygen ions through the electrolyte to the anode and react with hydrogen to generate water and electronic.

$$\text{Cathodic reaction: } \frac{1}{2}O_2 + 2e^- \leftrightarrow O^{2-} \tag{1}$$

$$\text{Anodic reaction: } H_2 + O^{2-} \leftrightarrow H_2O + 2e^- \tag{2}$$

$$\text{The overall reaction: } H_2 + \frac{1}{2}O_2 \leftrightarrow H_2O \tag{3}$$

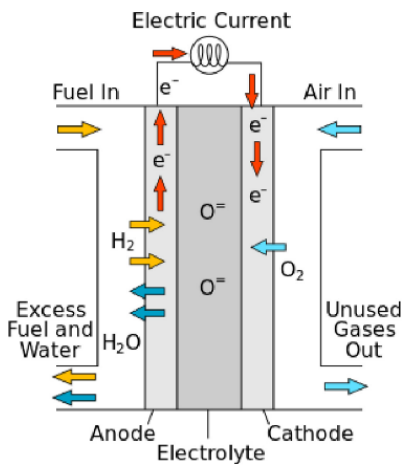

Fig.1 SOFC Schematic Diagram [6]

2.1. Electrochemical reaction

In order to establish the SOFC lumped model, the following assumptions are required:

1)The fuel gas is pure hydrogen

2)The gas is an ideal gas and uniformly distributed

3)Air is made up of 21% oxygen and 79% nitrogen

4)No heat loss

The open circuit voltage of SOFC single cell can be expressed by Nernst equation:

$$\mathrm{E} = E^0 + \frac{RT}{2F} ln \frac{P_{H2} P_{O2}^{0.5}}{P_{H2O}} \tag{4}$$

E^0 is a standard electric potential; R is the universal gas constant; F is Faraday constant; T is the operating temperature of SOFC; P_{H2} , P_{H2O}, P_{O2} are respectively hydrogen water vapor and oxygen partial pressure.

Standard electric potential E^0 has a linear relation with the battery temperature:

$$E^0 = 1.2586 - 0.000252\mathrm{T} \tag{5}$$

Under normal working conditions, the actual output voltage of SOFC is less than the output voltage V of open circuit due to the influence of activated polarization, concentration polarization and ohm polarization.

$$\mathrm{V} = \mathrm{E} - \eta_{ohm} - \eta_{con} - \eta_{act} \tag{6}$$

Because the electrode is different from the electrolyte material, the ohm polarization voltage caused by the resistance generated when the particle flow passes through the electrode and electrolyte can be calculated from the following formula [7, 9]:

$$\eta_{ohm} = \mathrm{J}R_{ohm} \tag{7}$$

J is the current density; R_{ohm} m resistance is the ohm.

$$R_{ohm} = \frac{\tau_{an}}{\sigma_{an}} + \frac{\tau_{ca}}{\sigma_{ca}} + \frac{\tau_{el}}{\sigma_{el}} + \frac{\tau_{int}}{\sigma_{int}} \tag{8}$$

τ_{an}, τ_{ca} , τ_{el}, τ_{int} anode, cathode, electrolyte and the thickness of the connection body; σ_{an} , σ_{ca} , σ_{el} , σ_{int} anode, cathode, electrolyte and connection of electrical conductivity.

Activation polarization is the most important cause of pressure drop, which is influenced by working temperature and pressure. Activation polarization consists of cathode activation polarization and anode activation polarization, which can be calculated by Butler-Volmer equation [8]:

$$\eta_{act,i} = \frac{RT}{F} sinh^{-1}\left(\frac{J}{2J_{0,i}}\right) = \frac{RT}{F} ln\left[\frac{J}{2J_{0,i}} + \sqrt{\left(\frac{J}{2J_{0,i}}\right)^2 + 1}\right] \tag{9}$$

$J_{0,i}$ is exchange current density.

Concentration polarization voltage is the voltage loss caused by the change in the concentration of the reaction gas, which can be calculated from the following formula [10]:

$$\eta_{con} = \frac{RT}{2F}\left(ln\left(\frac{P_{H2O,TPB}}{P_{H2O}}\frac{P_{H2,TPB}}{P_{H2}}\right) + ln\left(\frac{P_{O2}}{P_{O2,TPB}}\right)^{0.5}\right) \tag{10}$$

P_{H2O} , P_{H2}, P_{O2} and $P_{H2O,TPB}$, $P_{H2,TPB}$, $P_{O2,TPB}$ are water vapor, hydrogen and oxygen partial pressure in gas channels and partial pressure of three-phase interface.

2.2. Conservation of mass

The effective partial pressure of the gas in the flow passage can be determined by the ideal gas equation [11]:

$$\frac{dP_{H2}}{dt} = \frac{RT}{V_{an}}\left(q_{H2}^{in} - q_{H2}^{out} - q_{H2}^{r}\right) \tag{11}$$

$$\frac{dP_{H2O}}{dt} = \frac{RT}{V_{an}}\left(q_{H2O}^{in} - q_{H2O}^{out} - q_{H2O}^{r}\right) \tag{12}$$

$$\frac{dP_{O2}}{dt} = \frac{RT}{V_{cn}}\left(q_{O2}^{in} - q_{O2}^{out} - q_{O2}^{r}\right) \tag{13}$$

V_{an} is anode volume; V_{cn} is cathode volume; q_i^{in},q_i^{out},q_i^{r} is I gas entry, exit and to participate in the molar flow rate response (mol/s).

The molar flow of hydrogen involved in the reaction and outlet can be determined by the basic electrochemical relationship:

$$q_{H2}^{r} = 2K_r I \tag{14}$$
$$q_{H2}^{out} = K_{H2} P_{H2} \tag{15}$$

$K_r = \frac{N_0}{4F}$; I is the load current (A); N_0 is the number of single cells in series. K_{H2} is the valve molar constant of hydrogen. By arranging the above equation and applying Laplace transform to both sides of the equation, three partial pressures of gases can be obtained:

$$P_{H2} = \frac{1/K_{H2}}{1+\tau_{H2}s}\left(q_{H2}^{in} - 2K_r I\right) \tag{16}$$
$$P_{H2O} = \frac{1/K_{H2O}}{1+\tau_{H2O}s} 2K_r I \tag{17}$$
$$P_{O2} = \frac{1/K_{O2}}{1+\tau_{O2}s}\left(q_{O2}^{in} - K_r I\right) \tag{18}$$

$\tau_{O2} = \frac{V_{ca}}{K_{O2}RT}, \tau_{H2O} = \frac{V_{an}}{K_{H2O}RT}, \tau_{H2} = \frac{V_{an}}{K_{H2}RT}$ is respectively the time constant of hydrogen and oxygen, water vapor.

2.3. Thermodynamic conservation

Too low temperature leads to a decrease in SOFC efficiency, and too high temperature will cause irreversible damage. Therefore, the analysis of SOFC thermal balance is critical. During the establishment of SOFC lumped model, assuming that all components of the battery have the same temperature, the temperature change can be calculated through energy balance [12]:

$$\frac{dT}{dt} = \frac{1}{m_e \overline{C_p}}\left(\sum n_i^{in} C_{p,i}^{in}\left(T_{in} - T_{ref}\right) - \sum n_i^{out} C_{p,i}^{out}\left(T - T_{ref}\right) - 2K_r I \Delta\widehat{H_r^o} - VI\right) \tag{19}$$

m_e、$\overline{C_p}$ Is the mass and average specific heat of the electrode and interconnect; $C_{p,i}^{in}$ is the specific heat at the inlet of the gas i; $\Delta\widehat{H_r^o}$ is the specific heat of the reaction; V is the output voltage; T_{in} is gas inlet temperature.

2.4. Model construction

In this paper, the lumped model of SOFC is established based on mass conservation, thermodynamic conservation and electrochemical conservation on the MATLAB / Simulink software platform, as shown in Figure 2. The specific parameters of the mechanism model are determined by fitting with the actual experimental data. The fitting results are shown in Figure 12. This model can be used to analyze the steady-state and transient responses of SOFC.

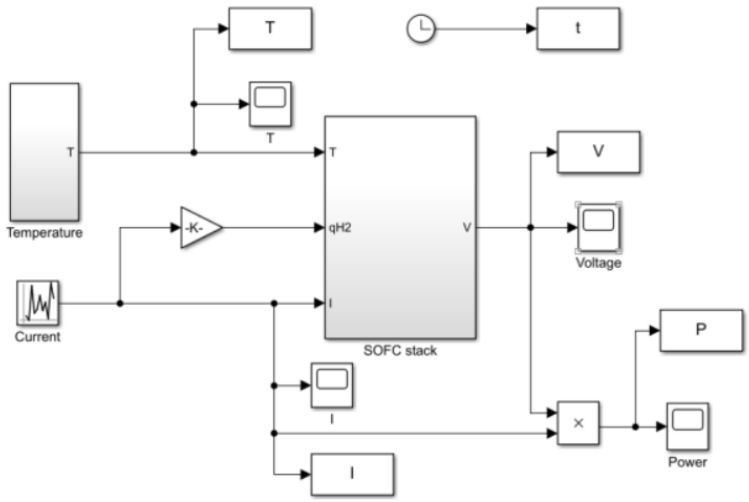

Fig.2 Lumped model of SOFC

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3. SOFC feature analysis

3.1. Steady-State characteristics

Fig.3 shows the characteristic curves of output voltage and current of single battery at different temperatures. As can be seen from the figure, the higher the temperature, the higher the output voltage. This phenomenon is relatively obvious under high current density, and the reason for this trend is similar to the influence of changing current density on output voltage. The activation polarization voltage and ohm polarization voltage decrease with the increase of temperature or load current [13].

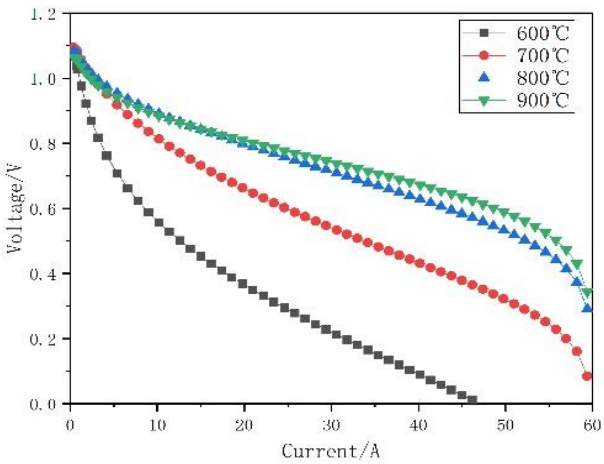


Fig.3 Volt-ampere characteristics of single battery at different temperatures

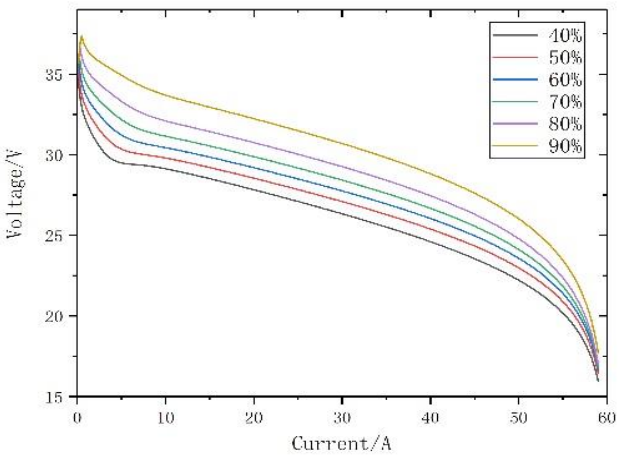


Fig.4 Stack volt-ampere characteristics at different fuel efficiencies

The impact of fuel efficiency on the SOFC stack output voltage is shown in Fig.4. When the load current is constant, the higher the fuel efficiency is, the higher the output voltage is. In order to maintain high efficiency and prevent fuel depletion, fuel efficiency is generally kept between 70% and 90%.

3.2. Dynamic characteristics

The step change of the load current within 300 seconds is shown in Fig.5. The lumped model is dynamically tested in the open loop state. The step change of the current causes the abrupt change of the voltage because the ohm polarization voltage follows the trend of the current

change. In the actual system operation, the voltage needs to be maintained in a stable state, so in the design of the controller, the current is generally used as a disturbance variable.

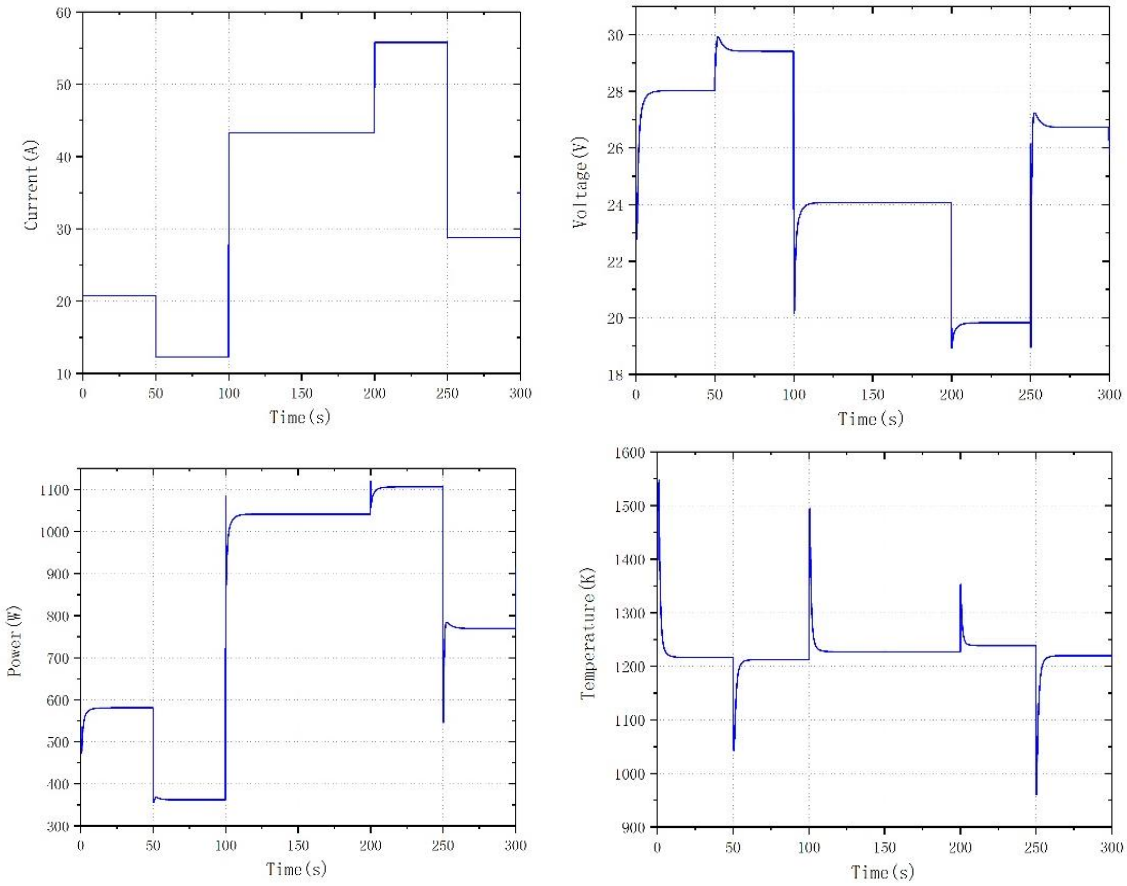


Fig.5 Influence of load change on voltage, power and temperature

4. Neural network modeling

The neural network does not need to establish complex mechanism model, and can fit arbitrary nonlinear model. It is convenient to study the dynamic characteristics of SOFC by using neural network. But it can only reflect the response of the system output to the input, not explain how it works.

4.1. BP neural network algorithm

BP neural network is a multi-layer feedforward neural network, which is characterized by forward signal propagation and error back propagation. BP neural network is composed of input layer, hidden layer and output layer. Its structure is shown in Fig.6. Where X is the system input, Y is the system output, and ω is the weight.

4.2. Optimization of BP neural network by genetic algorithm

The working principle of BP neural network is to achieve the optimal fitting through constant adjustment of weights, so the selection of weights has a great impact on the fitting accuracy. Genetic algorithm can be used to optimize the initial weight of BP neural network to improve the fitting accuracy. The optimization process is shown in Fig.7.

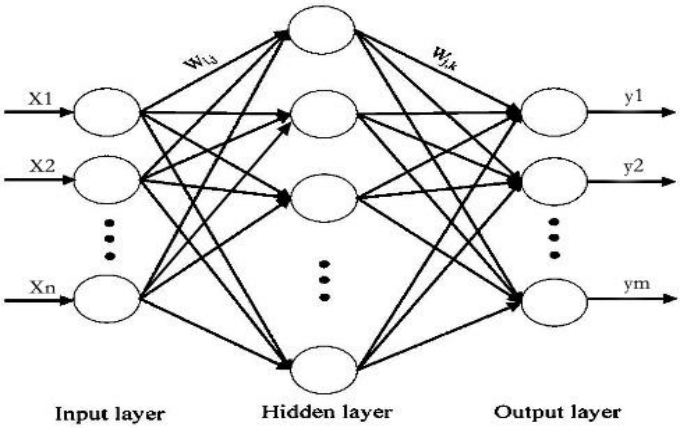


Fig.6 BP neural network structure

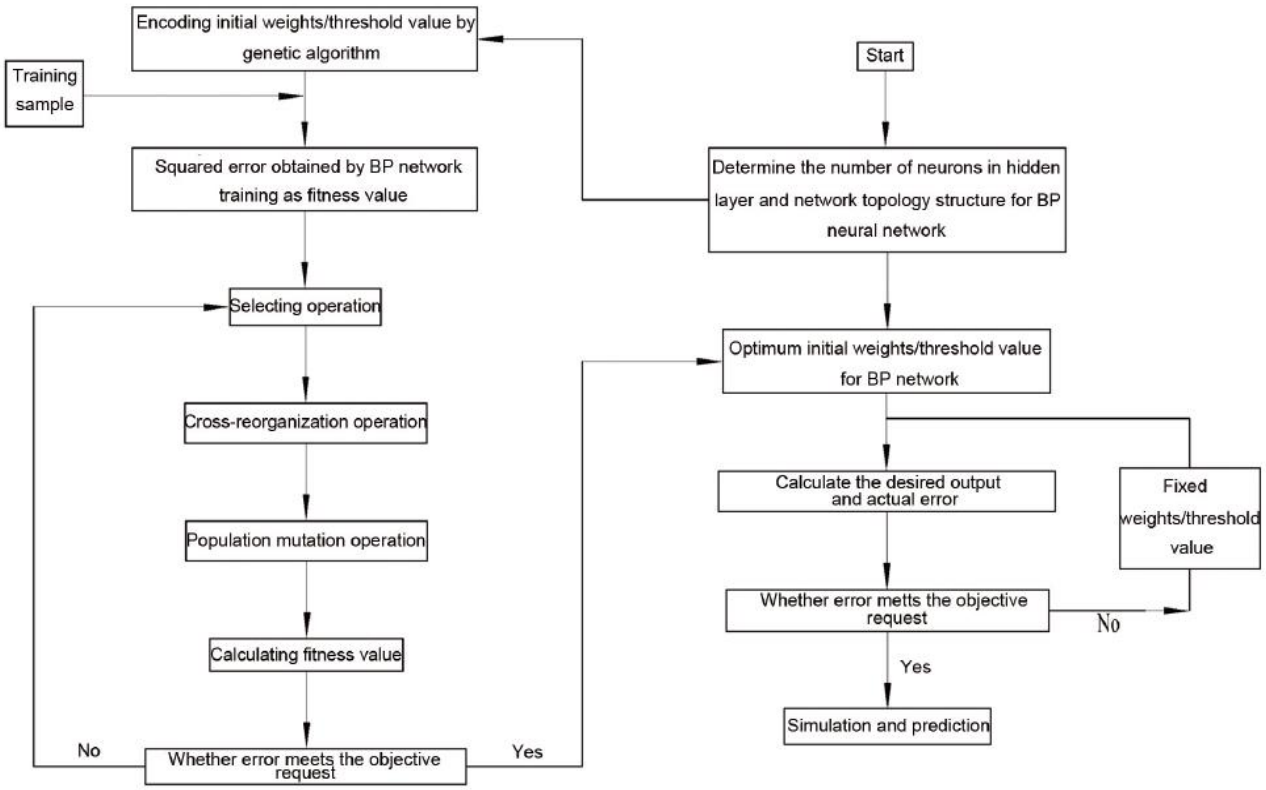


Fig.7 Genetic algorithm optimization BP neural network flow [14]

4.3. Structure determination and fitting

GE-BP of three - layer network structure is selected. The input layer has four input parameters, namely, current, hydrogen flow rate, air flow rate and temperature. Theoretically, any nonlinear model can be fitted with 3 neurons in the hidden layer of the neural network, and different numbers of neurons are selected for simulation. Among them, 10 neurons in the hidden layer have the best fitting effect, so the network structure is set as 4-10-1. According to literature [15], the activation function of neurons was determined. Hyperbolic tangent S-type activation function (Sigmoid) was selected for the hidden layer and linear activation function (Purelin) was selected for the output layer. References for specific steps of genetic algorithm optimization [16].

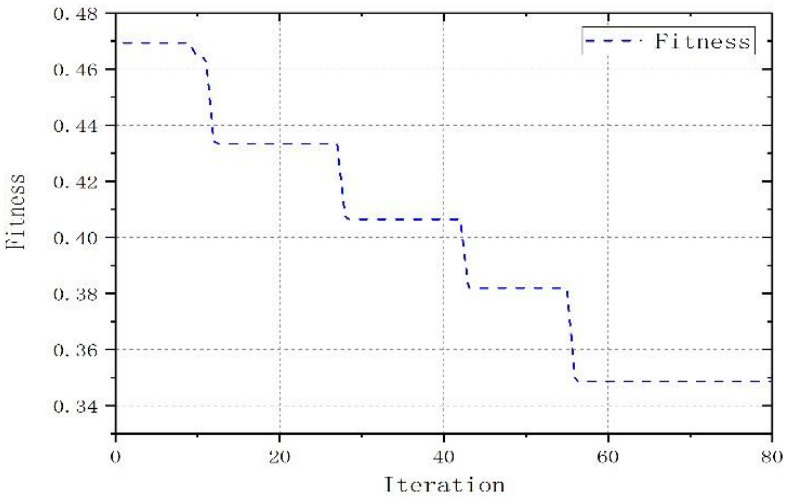
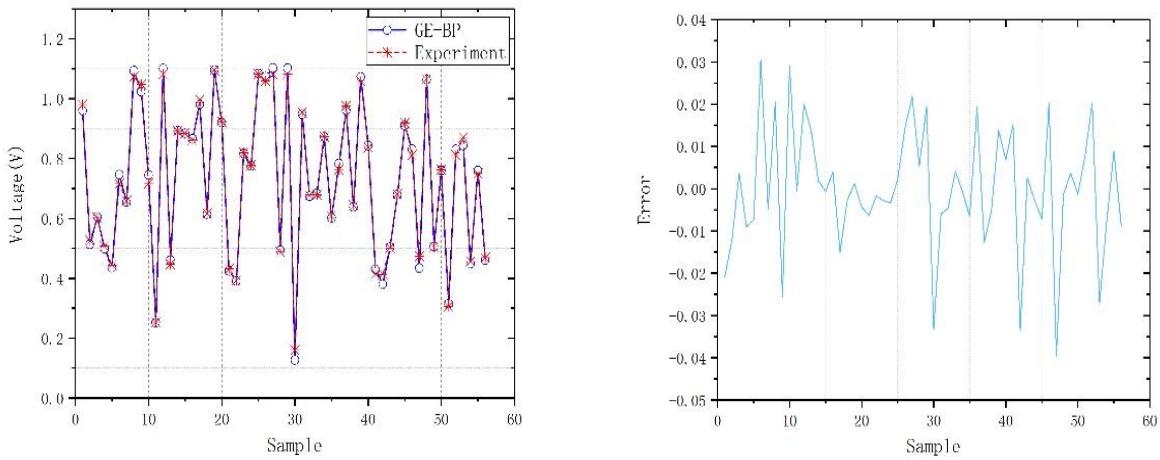


Fig.8 Variation of fitness of genetic algorithm with iteration

GE-BP was used to train and test the data generated by the lumped model. The iterative optimization of genetic algorithm was shown in Fig.7, and the maximum number of iterations was 80. GE-BP test data and experimental data are shown in Fig.9.a, and the fitting error is shown in Fig.9.b. GE-BP can fit the experimental data well, and the fitting error is within 5%, which meets the experimental requirements.



a) b)

Fig.9 GE-BP test data and errors

4.4. Prediction analysis and discussion

In order to verify the performance of genetic algorithm to optimize the BP neural network is better than not to optimize the BP neural network, this paper used two methods of lumped model of experimental data fitting, fig.10.a fitting curve shows the two methods, GE - BP can very good fitting the experimental data, the BP neural network in low load shedding fitting effect is poorer, high load power flow fitting is good. Fitting error as shown in fig.10.b, GE - BP fitting error is within 5% of the whole, and the BP neural network in low load shedding fitting error was 15%, while in high load power flow also remain in the 5% range, but relative to the overall, based on the genetic algorithm to optimize the BP neural network is better than not optimized BP neural network. Therefore, this paper selects BP neural network optimized by genetic algorithm to predict SOFC performance.

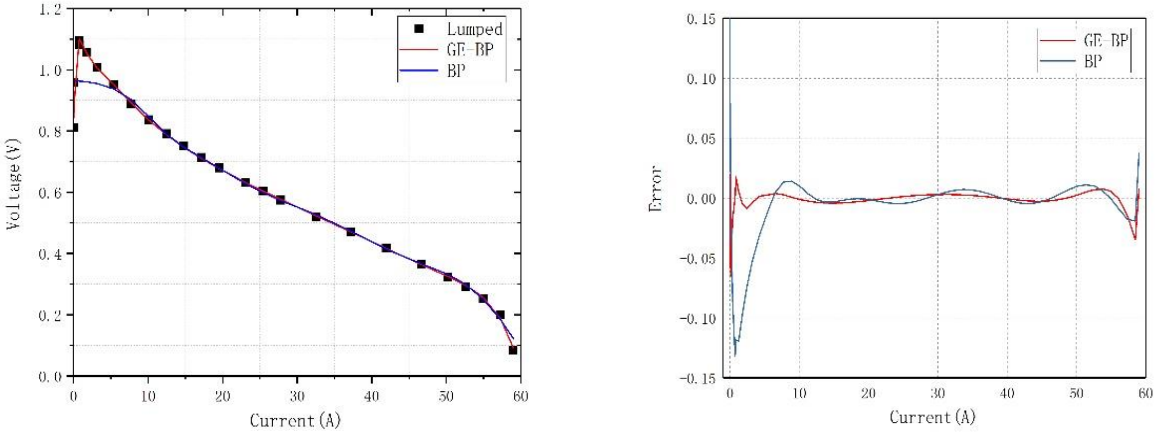


Fig.10 Comparison of predicted performance between GP-BP and BP

4.5. Predictive analysis

The effect of temperature on SOFC performance can be clearly seen through the steady-state analysis of 2.1. SOFC is a nonlinear, multivariable coupling system that maintains gas flow at a fixed fuel efficiency rate in order to predict the impact of a variable on SOFC performance. The training data temperature is composed of four different temperatures, namely 973K, 1073K, 1173K and 1273K. The fitting and prediction results are shown in Fig.11. When the temperature is 973K, the neural network data can well fit the experimental data. In order to verify the predictive performance of the neural network, the volt-ampere characteristics curves of SOFC at 1023K and 1223K without training are simulated. The experimental results show that the BP neural network based on genetic algorithm optimization can predict the SOFC performance well.

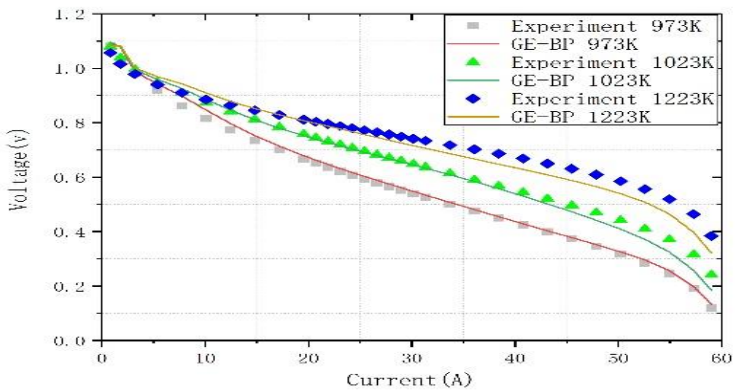


Fig.11 GE-BP predicts SOFC performance at different temperatures

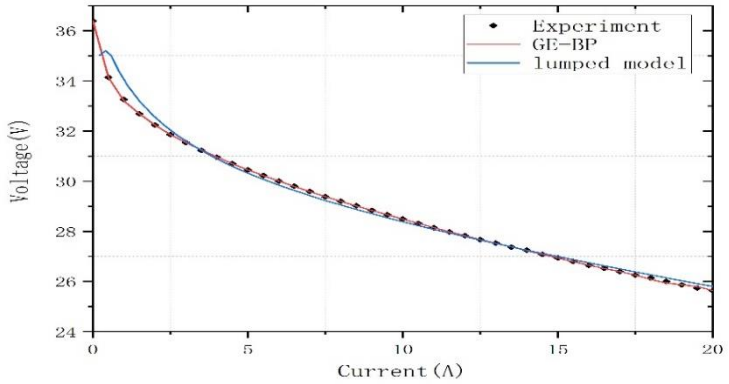


Fig.12 GE-BP and lumped model fitting comparison of actual test data

Through the fitting comparison of actual test data between GE-BP and lumped model (as shown in Fig. 12), it can be found that compared with lumped model, neural network model has higher fitting accuracy and is more suitable for SOFC performance prediction.

5. Conclusion

In this paper, two different modeling methods are proposed, namely mechanism modeling and neural network modeling. The lumped model needs complex mathematical formulas and many assumptions. The fitting results have a certain deviation from the reality, but it can well explain the internal principle and change dynamics of SOFC. The steady-state and transient response of SOFC can be analyzed through the lumped model. The neural network model has high fitting accuracy and can also predict the performance of SOFC, but it can not explain the change mechanism.

Lumped model and neural network model have their own advantages and disadvantages. After analyzing the advantages and disadvantages of the two models, they can be used in appropriate situations. If accurate fitting of experimental data is not required, but the overall trend of SOFC performance curve can be followed, lumped model can be selected to facilitate the design of controller in the later stage. If a large amount of experimental data is available, a neural network model can be selected to predict SOFC performance within the data range.

In this paper, a 4-10-1 structure neural network is selected to predict SOFC performance based on four different parameters, including temperature, hydrogen flow rate, air flow rate and load current. The BP neural network based on genetic algorithm is verified with high accuracy and unoptimized BP neural network, and the BP neural network optimized by genetic algorithm is used to predict the volt-ampere characteristic curve of SOFC at different temperatures. The simulation results are very close to the experimental results, which means that this method can predict the performance of SOFC in various environments.

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