Modeling and Simulation of the Electrical Characteristic of Solid Oxide Fuel Cells

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Abstract. Solid oxide fuel cell (SOFC) is a new type of clean energy power generation device. In this paper, the SOFC model is established by introducing adjustable parameters, considering the voltage loss of concentration polarization, activation polarization and ohmic polarization, combined with the ideal gas state equation and the law of mass conservation. The simulation results show that the model can accurately reflect relationship between the input molar flow of each gas and the output characteristics of SOFC single battery, and adjustable parameters can be adjusted according to actual situation so the model has certain flexibility.

1. Introduction
Fuel cell is the fourth generation of new power generation technology after hydropower, thermal power and nuclear power. SOFC has a series of advantages including high energy efficiency, quiet and pollution-free, wide range of fuel sources, all-solid state, etc. However, SOFC is not widely used due to its high cost and transportation difficulties [1]. At the same time, SOFC's internal structure and chemical reaction are complex, and it is easy to be affected by external factors, making the SOFC's output performance difficult to meet the specified requirements. Therefore, the research on SOFC modeling has become the focus of scholars [2].

In foreign countries, Andrew J.Slippey established a new component model of planar SOFC stack and partial oxidation (POX) converter in 2009. By introducing new dynamics model and power distribution model, the existing and new models were updated and transformed, providing a basis for the development of future hybrid control schemes [3]. In 2010, Yousuke Iida established a model based on SOFC multi-level functional block by applying physical principles. This model reflects the dynamic characteristics of power generation relying on load fluctuation, and can also estimate the internal temperature of the module. For researchers, they can also arbitrarily change and expand the structure of the module to establish the corresponding model [4]. In 2016, Shenglong Yu, Tyrone Fernando and Herbert H.C.I. analyzed the performance of SOFC in a complex power system composed of different types of synchronous motors, established a mathematical model for practical tubular solid oxide fuel cells, and designed a state estimator for tracking and predicting the internal behavior of SOFC [5]. In China, the modeling of SOFC is also gradually deepened. In 2010, considering that the electrochemical reaction in the process of high temperature will affect battery performance of solid materials, and battery temperature shows the characteristics of strong nonlinear, Chuan-pei xu established t-s fuzzy model for battery temperature of SOFC. This battery temperature...
model can accurately fit the mapping characteristic of cell dynamic response [6]. In 2011, Ma teng discovered the electrical coupling phenomenon of SOFC by analyzing the measured data of SOFC, established the corresponding identification model with genetic algorithm, and proposed a new modeling strategy [7]. In 2012, Wu dazhong applied particle swarm optimization radial basis neural network algorithm to identifying SOFC single-cell system and obtained SOFC identification model [8]. In 2016, Hu aosheng from Nanjing University of Technology, applied Dusty-gas model to simulating the mass transfer process and established the anode microscopic model of an solid oxide fuel cell. This model can accurately describe the anode performance of a SOFC [9].

The existing SOFC models are mostly idealized models established under certain external conditions, which can accurately reflect the SOFC output performance under certain external conditions. However, as long as the external conditions change, such models will no longer be applicable [10,11]. In this paper, considering three kinds of polarized voltages loss, an SOFC model with two adjustable parameters $Q_f$ and $M$ is established, where $Q_f$ is the utilization rate of hydrogen and $M$ is the ratio of hydrogen to oxygen. The two parameters of the model can be adjusted according to actual operation condition of SOFC conduct corresponding adjustments. The more flexible mathematical models of SOFC can more accurately reflect the actual relationship between input and output of SOFC.

2. Establishment a common model for SOFC

The output voltage of SOFC single cells is about 0.8v. In order to obtain higher voltage, multiple SOFC single cells need to be stacked together in series or parallel to form a pile with different voltage sizes to supply power for external circuits. Regardless how the stack ends up, the SOFC single battery is the most basic building block. The output voltage of a single battery is shown in Eq.1.

$$U_{cell} = E - U_{act} - U_{con} - U_{ohmic}$$ (1)

where, $E$ is generated electromotive force; $U_{act}$, $U_{con}$ and $U_{ohmic}$ are respectively activation polarization voltage, concentration polarization voltage and ohmic polarization voltage.

The generated electromotive force is the open circuit voltage of the battery, which is mainly affected by the performance of reactants. It can be expressed with Nernst equation.

$$E = E^0 + \frac{RT}{2F} \ln \left( \frac{P_{H_2}}{P_{H_2O}} \right)$$ (2)

where, $P_{H_2}$, $P_{O_2}$ and $P_{H_2O}$ are partial pressures of reactants. $R$ is universal gas constant; $F$ is Faraday constant; $E^0$ is electromotive force due to Gibb’s free energy, usually $E^0 = 1.1$ V; $T$ is real-time temperature of the battery.

The activation polarization voltage is a part of the energy consumed in the electrochemical reaction process to overcome the activation energy to maintain the reaction. Activation polarization voltage can be expressed with Butler-Volmer equation.

$$U_{act} = \frac{RT}{F} \arcsinh \left( \frac{I}{2I_0} \right) = \frac{RT}{F} \ln \left[ \frac{I}{2I_0} + \sqrt{1 + \left( \frac{I}{2I_0} \right)^2} \right]$$ (3)

where, $I_0$ is exchange current; $I$ is battery current; $T$ is real-time temperature.

Concentration polarization voltage is the voltage that loss due to the instability of the flow caused by the change of the concentration of the reactant nearby when the reaction gas on the battery electrode is consumed due to chemical reaction. Concentration polarization voltage can be calculated by Eq.(4) with limiting current $I_L$.

$$U_{con} = \frac{RT}{nF} \ln \left( 1 - \frac{I}{I_L} \right)$$ (4)

Different from the polarization mentioned above, the ohmic polarization is caused by the impedance between the ion flow in the electrolyte and the electron flow in the electrode material,
which is the inherent property of the battery. The battery performance can only be changed by changing the electrolyte material or the thickness of the anode and the cathode. And as shown in Eq. (5), the ohmic polarization is easily affected by the temperature.

\[
U_{\text{ohmic}} = \left\{ \lambda \exp \left[ \beta \left( \frac{1}{T_0} - \frac{1}{T} \right) \right] \right\} l = r l
\]

where, \( T_0 \) is initial temperature of the battery; \( \lambda = 0.2 \ \Omega \) and \( \beta = -2870 \ \text{k} \) are battery constant coefficients; \( r \) is the equivalent resistance of a single battery including ion and electronic resistance.

3. Establishment of adjustable parameter model for SOFC

3.1. Calculation of partial pressure of gas in SOFC

Under ordinary conditions, the physical behavior of most actual gases is close to that of ideal gases, which can be described by the ideal gas state equation.

\[
P V = n R T
\]

where, \( P \) is pressure of an ideal gas; \( V \) is volume of an ideal gas; \( n \) is the number of moles of gas; \( R \) is universal gas constant.

All kinds of gases inside SOFC can be regarded as ideal gases. The partial pressure of all kinds of gases inside the battery can be solved by applying Eq. (6). The derivative of both sides of the above equation with respect to time can be obtained Eq. (7).

\[
\frac{d}{dt} p = \frac{R T}{V} \times \frac{d}{dt} n
\]

Applying the law of mass conservation, we can obtain Eq. (8).

\[
\frac{d}{dt} n = n_{in} - n_{out} - n^r
\]

where, \( n_{in} \) for the gas in the type of input molar flow; \( n_{out} \) for the gas output of the molar flow; \( n^r \) the gas consumption for electrochemical reaction molar flow.

Because SOFC is a high-temperature fuel cell, the external fuel gas will undergo reforming reaction in SOFC to generate hydrogen-rich gas. Therefore, only the electrochemical reaction of hydrogen needs to be considered. Therefore, the internal pressure of SOFC can be calculated according to Eq. (9).

\[
\begin{align*}
\frac{d}{dt} p_{H_2} &= \frac{RT}{V_{H_2}} (n_{in}^{H_2} - n_{out}^{H_2} - n_{H_2}^r) \\
\frac{d}{dt} p_{O_2} &= \frac{RT}{V_{O_2}} (n_{in}^{O_2} - n_{out}^{O_2} - n_{O_2}^r) \\
\frac{d}{dt} p_{H_2O} &= \frac{RT}{V_{H_2O}} (n_{in}^{H_2O} - n_{out}^{H_2O} - n_{H_2O}^r)
\end{align*}
\]

where, \( V_{H_2}, V_{O_2}, \) and \( V_{H_2O} \) respectively represent the volumes of hydrogen, oxygen, and water vapor in SOFC single cell.

3.2. Definition of adjustable parameters in SOFC

In general, the hydrogen participating in the reaction cannot be fully reacted. The low utilization rate of hydrogen will reduce the power generation efficiency of SOFC and fail to meet the actual power generation demand. However, hydrogen overutilization can lead to depletion of hydrogen at the inlet of the fuel channel, making it difficult to maintain SOFC’s continuous power generation. Therefore, in this paper, the hydrogen utilization rate of \( Q_f \) is studied as an adjustable parameter, which is defined as follows.

\[
Q_f = \frac{n_{H_2}^r}{n_{in}^{H_2}}
\]
where, \( n_{\text{H}_2}^{\text{in}} \) is the molar flow consumed in an electrochemical reaction; \( n_{\text{H}_2}^{\text{in}} \) is the input molar flow of hydrogen.

At the same time, excessive pressure difference between the gas in fuel channel and air channel will cause fission of the two side of electrode of SOFC. Long-term operation under this condition will not only affect the life of SOFC, but also cause explosion of the battery. Therefore, in practical operation, instead of using ideal ratio of hydrogen and oxygen, it is necessary to appropriately increase the share of oxygen to balance electrochemical reaction inside SOFC. The ratio \( M \) of hydrogen to oxygen is regarded as another adjustable parameter, which is defined as follows.

\[
M = \frac{n_{\text{H}_2}^{\text{in}}}{n_{\text{O}_2}^{\text{in}}}
\]  

where, \( n_{\text{O}_2}^{\text{in}} \) is the input molar flow of oxygen.

The output molar flow of each gas is related to the gas mole threshold constant and the partial pressure of the gas in the battery. The output molar flow of each gas can be obtained from literature [2], as shown in Eq.(12).

\[
\begin{align*}
    n_{\text{H}_2,\text{O}_2}^{\text{out}} &= K_{\text{H}_2,\text{O}_2}P_{\text{H}_2,\text{O}_2}; \\
    n_{\text{O}_2}^{\text{out}} &= K_{\text{O}_2}P_{\text{O}_2}; \\
    n_{\text{H}_2,\text{O}_2}^{\text{O}_2} &= K_{\text{H}_2,\text{O}_2}P_{\text{H}_2,\text{O}_2}
\end{align*}
\]  

where, \( K_{\text{H}_2,\text{O}_2}, K_{\text{O}_2}, K_{\text{H}_2,\text{O}_2} \) for the gas mole threshold constants, \( K_{\text{H}_2} = 0.834 \), \( K_{\text{O}_2} = 2.52 \), \( K_{\text{H}_2,\text{O}_2} = 0.281 \).

Substitute Eq.(10) –Eq.(9), we can yield the mathematical relationship between the input molar flow of each gas in SOFC and the partial pressure of each gas given in Eq.(13).

\[
\begin{align*}
    \frac{d}{dt}p_{\text{H}_2} &= \frac{RT}{V_{\text{H}_2}}(n_{\text{H}_2}^{\text{in}} - K_{\text{H}_2}P_{\text{H}_2} - Q_{\text{f}}n_{\text{H}_2}^{\text{in}}) \\
    \frac{d}{dt}p_{\text{O}_2} &= \frac{RT}{V_{\text{O}_2}}(\frac{n_{\text{H}_2}^{\text{in}}}{M} - K_{\text{O}_2}P_{\text{O}_2} - \frac{1}{2}Q_{\text{f}}n_{\text{H}_2}^{\text{in}}) \\
    \frac{d}{dt}p_{\text{H}_2,\text{O}_2} &= \frac{RT}{V_{\text{H}_2,\text{O}_2}}(n_{\text{H}_2,\text{O}_2}^{\text{in}} - K_{\text{H}_2,\text{O}_2}P_{\text{H}_2,\text{O}_2} + Q_{\text{f}}n_{\text{H}_2}^{\text{in}})
\end{align*}
\]

By substituting Eq.(5) –Eq.(5) into Eq.(5), the output voltage of SOFC single cell can be obtained. Combining Eq.(13) with Eq.(1), we can obtain the mathematical relationship between the input molar flow of hydrogen, the input molar flow of water vapor and the output voltage of SOFC single cell, and the SOFC model with two adjustable parameters.

4. Experimental simulation and analysis
In the established adjustable parameter model of SOFC, the output voltage of SOFC single battery is related to the input molar flow of hydrogen and water vapor. In order to discuss the relationship between one single input variable (\( n_{\text{H}_2}^{\text{in}} \) or \( n_{\text{H}_2}^{\text{in}} \)) and the output voltage of SOFC single battery, another input variable (\( n_{\text{H}_2}^{\text{in}} \) or \( n_{\text{H}_2}^{\text{in}} \)) needs to be fixed.

When \( Q_{\text{f}} = 85\% \), \( M = 1.2 \), \( n_{\text{H}_2,\text{O}_2}^{\text{in}} = 1.5 \), the relationship between the hydrogen input molar flow and the SOFC single cell output voltage is shown in Fig.1, and the relationship between the hydrogen input molar flow and the power of SOFC single cell is shown in Fig.2.

It can be seen from Fig.1 that when the hydrogen input molar flow increases from 0 to 0.283, the output voltage of SOFC single battery increases from 0.8V to 0.832V. As the hydrogen input molar flow continues to increase after that, the output voltage of the SOFC single cell continues to decrease. It indicates that there is an optimal input molar flow of hydrogen in SOFC system to maximize the output voltage of SOFC single battery.

Fig.2 shows that when the hydrogen input molar flow increases from 0 to 3.08, the power of SOFC single battery increases from 0W to 2.28W. The power of SOFC single battery decreased slowly from 2.28W when the hydrogen input molar flow increased from 3.08 to 6. The same varying tendency of curves in Fig.1 and Fig.2 indicates that there is an optimal value of hydrogen input molar flow to
maximize the power of SOFC single cells. But, the maximum output voltage and maximum power of SOFC single battery do not appear at the value of hydrogen input molar flow. That means hydrogen input molar flow affects the output current of SOFC.

Fig. 1 and Fig. 2 reflects the electrochemical reaction process of SOFC precisely. At the initial generation stage of SOFC, the hydrogen input molar flow keep increasing to the amount of material consumed to maintain the equilibrium of electrochemical reaction. During this period, increasing the input molar flow of hydrogen will increase the Nernst electromotive force of the battery, thus increase the output voltage and power of the battery. After a period of continuous power generation, the electrochemical reaction inside SOFC has reached equilibrium. Increasing the input molar flow of hydrogen will not only fail to improve the output voltage of the battery, but also affect the partial pressure of the gas inside the battery, resulting in a reduction in the output voltage and power of the battery.

When $Q_f = 85\%$, $M = 1.2$, $n_{H_2}^{in} = 1.5$, the relationship between the water vapor input molar flow and the output voltage of SOFC single battery is shown in Fig. 3. The relationship curve between the water vapor input molar flow and the power of SOFC single battery is shown in Fig. 4.

Fig. 3 shows that when the water vapor input molar flow increased from 0 to 1.8, output voltages of SOFC single battery decreased from 1.2V to 0.72V, showing a rapid decline trend. The SOFC single cell output voltage drops slowly as the water vapor input molar flow continues to increase from 1.8. It shows that the water vapor input molar flow is negatively correlated with the output voltage of SOFC single cell.

The same varying tendency of curves in Fig. 3 and Fig. 4 indicates that the power of SOFC single cells continues to decrease as the vapor input molar flow increases. The reasons for this situation are
that with the increasing of water vapor input molar flow, the battery internal water vapor pressure increases gradually. Thus the Nernst electromotive force of the battery reduces and affects the output performance of the battery.

5. Conclusions
In this paper, SOFC adjustable parameter model is established, and the input-output characteristic of SOFC single battery is study by simulation. The comparisons and analysis of Fig.1 to Fig.4 indicate that when $Q_f=85\%, \ M=1.2, \ \text{H}_2\text{O}^{\text{in}}=1.5$, the output voltage of SOFC single cell can be maximized at $\text{H}_2^{\text{in}}=0.283$, when $Q_f=85\%, \ M=1.2, \ \text{H}_2\text{O}^{\text{in}}=1.5$, the power of SOFC single cell can be maximized at $\text{H}_2^{\text{in}}=3.08$ and reducing the water vapor input molar flow will increase the output voltage and power of SOFC single cells.

The study in this paper shows that in the actual SOFC single cell system, when the water vapor input molar flow is fixed at a small value, there is an optimal hydrogen input molar flow to achieve the optimal output performance (output voltage or power) of SOFC single cell, which lays a foundation for the controller design.

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