Modeling and simulation of solid oxide fuel cell under different environmental conditions

HE Junneng, QIAO Runpeng, LIANG Qianchao, YANG Fan
College of Naval Architecture and power, Naval University of Engineering, Wuhan Hubei 430033, China
e-mail address:hjn19960201@163.com

Abstract. This article firstly based on Matlab/Simulink software to model and simulate the solid oxide fuel cell (SOFC), obtain the SOFC volt-ampere characteristic curve, and verify the correctness of the model; secondly, according to the existing 1KW SOFC in the laboratory, the stack has determined the initial parameters of the simulation, simulated the effects of the air inlet pressure and the nitrogen-oxygen ratio on the SOFC output voltage and electrical efficiency, and compared the analysis with the fuel inlet pressure. Finally, the conclusion is drawn: air inlet the increase in pressure can significantly increase the output voltage and electrical efficiency of the stack, and the increase in the oxygen content of the cathode intake increases the output power of the stack.

1. Introduction

The traditional use of fossil energy such as thermal power plants has the disadvantage of low energy conversion efficiency, and the excessive use of fossil energy has brought about a serious global energy crisis and environmental pollution, especially in developing countries such as China and India [1]. Fuel cells are not subject to the "Carnot cycle" and their energy efficiency is much higher than that of conventional heat engines, usually between 60% and 80% [2, 3]. Therefore, if SOFC is widely used in industrial power generation and other fields, it will greatly improve the utilization rate of energy, thus saving energy and protecting the environment; at the same time, SOFC can solve the problems of difficult power delivery, use and maintenance in remote areas; furthermore, if SOFC can be applied underwater, it will have a significant impact on the modernization of China's national defence. At present, many experts and scholars have carried out a lot of research on the relevant performance of SOFC. Zhu Runkai [4].et al. discussed the output performance of SOFC under the conditions of different flow rates, different pressures and different temperatures of the fuel. Zhao [5].et al. first established a SOFC power generation system based on an Aspen Plus simulation environment, using coal bed methane (CBM) as the anode fuel, and analysed the effect of different CBM concentrations on the power generation efficiency of SOFC. Sadeghi [6].et al. analysed a three-generation SOFC-based system in which the waste heat from SOFC exhaust gas is recovered for cooling and heating through an adsorption refrigeration system and heat exchanger. Irshad [7].et al. highlight research advances in the field of high temperature SOFC, discussing the impact of different types of conventional and innovative materials, as well as SOFC components (electrolyte anodes, cathodes, interconnects and sealing materials) on SOFC output performance.

There have been many studies on how to improve the catalytic performance of SOFC anodes, reduce carbon build-up in the stack and the effect of fuel flow on stack performance, but relatively little research has been done on the effect of air inlet pressure and fuel inlet pressure on stack...
performance. In this paper, a mathematical model of SOFC based on Matlab/Simulink software is developed, and the effects of air inlet pressure, nitrogen-to-oxygen ratio and fuel inlet pressure on the performance of SOFC are investigated through simulations, which provide theoretical support for the application of solid oxide fuel cells in industry and other fields.

2. Modular modelling

Assumptions
In this paper, the following assumptions are made when modelling the SOFC dynamics.
- All gases are ideal
- The heat exchange between the system and the outside world is ignored
- The reforming reaction and the water-gas replacement reaction are in equilibrium
- The temperature, gas components and pressure in the system are uniformly distributed
- The system is modelled using centralised parameters

Pre-reformer model
In the pre-reformer, which consists mainly of the reforming reaction of methane and the water-gas replacement reaction, the chemical reaction equations are as follows \(^{(8)}\):

\[
\begin{align*}
CH_4 + H_2O &\leftrightarrow CO + 3H_2 \quad (1) \\
CO + H_2O &\leftrightarrow CO_2 + H_2 \quad (2)
\end{align*}
\]

From the equation for conservation of mass it follows that \(^{(9)}\):

\[
\frac{PV_{re}}{RT_1} \frac{dx_{n,i}}{dt} = Q_{n_{6,i}} - Q_{n_{6,j}} + \overline{R}_{re,i} \quad (i \in [CH_4, CO, CO_2, H_2, H_2O]) \quad (3)
\]

\[
\overline{R}_{re} = [-r_{re1}, r_{re1} - r_{re2}, r_{re2}, 3r_{rel} + r_{re1}, 3r_{rel} - r_{re2}] \quad (4)
\]

\(P_1\) is the average pressure inside the pre-reformer, \(V_{re}\) is the volume of the pre-reformer, \(R_1\) is the average temperature of the pre-reformer, \(R\) is the universal gas constant, \(E\) is the molar mass fraction of the exit gas \((8.314 J \cdot mol^{-1} \cdot K^{-1})\), \(x_{n,j}\) is the molar flow rate of the inlet gas \(i\), \(Q_{n_{i,j}}\) is the molar flow rate of the outlet gas \(i\), \(\overline{R}_{re,j}\) is the molar flow rate of the gas \(i\) consumed in the pre-reformer for reforming and water-gas replacement reactions, \(r_{re1}\) represents the reforming rate of methane, and \(r_{re2}\) represents the replacement rate of carbon monoxide.

Assuming that the reforming reaction and the water-gas replacement reaction have reached equilibrium, the equilibrium constants can be expressed as \(^{(10)}\):

\[
\begin{align*}
K_r &= \exp\left( A_{1T_5^4} + B_{1T_5^3} + C_{1T_5^2} + D_{1T_5} + E_1 \right) \quad (5) \\
K_s &= \exp\left( A_{2T_5^4} + B_{2T_5^3} + C_{2T_5^2} + D_{2T_5} + E_2 \right) \quad (6)
\end{align*}
\]

where \(K_r\) and \(K_s\) are the equilibrium constants for the reforming and water-gas replacement reactions, respectively.

Anode model
The hydrogen produced by methane in the pre-reformer reaches the anode and reacts with the oxygen ions transmitted from the cathode to produce water and generate electrons that are transported to the external circuit. The reaction equation is as follows.

\[
H_2 + O^{2-} \rightarrow H_2O + 2e^- \quad (7)
\]

At this point the anode channel is a mixture of methane, hydrogen, water, carbon monoxide and carbon dioxide, and according to the equation for conservation of mass there is:
where $P$ is the anode outlet gas pressure, $T$ is the stack temperature, $V$ is the anode volume, $x$ is the molar fraction of the anode outlet gas, $m$ is the molar flow rate of the anode outlet gas, $r_1$ is the reforming reaction rate, $r_2$ is the water-gas replacement reaction rate and $r_3$ is the electrochemical reaction rate.

**Electrochemical model**
The actual voltage of a fuel cell monolith can be represented by the following equation.

\[
\eta_{f} = E - \eta_{\text{ohmic}} - \eta_{\text{conc}} - \eta_{\text{act,a}} - \eta_{\text{act,c}}
\]

Where $E$ is the stack ideal reversible voltage, $\eta_{\text{ohmic}}$ is the ohmic polarization, $\eta_{\text{conc}}$ is the differential concentration polarization, $\eta_{\text{act,a}}$ is the anodic activation polarization and $\eta_{\text{act,c}}$ is the cathodic activation polarization. According to the Nernst equation, the ideal reversible voltage of the reactor is expressed as [11]:

\[
E = E^0 + \frac{RT}{2F} \ln \left( \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \right)
\]

\[
E^0 = 1.2723 - 2.7645 \times 10^{-4} T
\]

where $E^0$ is the standard electric potential, $p_{H_2}$ is the pressure of hydrogen at the anode outlet, $p_{O_2}$ is the pressure of oxygen at the cathode inlet and $T$ is the temperature of the reactor.

**Temperature model**
According to the above assumptions, neglecting the heat exchange between the reactor and the outside world, the conservation of energy equation yields [12]:

\[
C_{cell} \frac{dT}{dt} = Q_{s5} \sum_j (X_{5,j} \tilde{h}_{5,j}) + Q_{s2} \sum_i (X_{2,i} \tilde{h}_{2,i}) - Q_{s6} \sum_j (X_{6,j} \tilde{h}_{6,j}) - \sum_i Q_i - P_{cell} + \sum Q_k
\]

where $i \in [CH_4, CO, CO_2, H_2, O_2]$, $j \in [N_2, O_2]$, $k = 1, 2, 3$, $C_{cell}$ is the reactor gas heat capacity, $\tilde{h}_{5,j}$ is the enthalpy of the SOFC cathode inlet gas, $\tilde{h}_{6,j}$ is the enthalpy of the cathode outlet gas, $Q_{s5}$ is the molar flow rate of the cathode inlet gas, $Q_{s6}$ is the molar flow rate of the cathode outlet gas, $\tilde{h}_{2,j}$ is the enthalpy of the anode inlet gas, $\tilde{h}_{4,j}$ is the enthalpy of the anode outlet gas, $Q_i$ is the heat of reforming reaction, $Q_2$ is the heat of water-gas replacement reaction and $Q_3$ is the heat of electrochemical reaction.
3. Performance analysis

According to the SOFC simulation model established above, combined with the existing 1KW SOFC test system in the laboratory, the initial parameters of the SOFC simulation model in this paper are shown in Table 1 below.

| Parameters                          | Unit | Numerical values            |
|-------------------------------------|------|----------------------------|
| Numerical fuel import composition  | —    | 100% CH₄                   |
| Fuel Inlet Flow                     | mol·s⁻¹ | 2.75 × 10⁻³             |
| Air import composition xₓₙₙ       | —    | 79% N₂ + 21% O₂            |
| Air inlet flow                      | mol·s⁻¹ | 2.37 × 10⁻²              |
| Fuel inlet pressure                 | Pₚ   | 1.013 × 10⁴               |
| Air inlet pressure                  | Pᵣ   | 1.013 × 10⁸               |
| Fuel inlet temperature             | Tᵣ   | K                         |
| Air inlet temperature              | Tᵣ   | K                         |
| SOFC input current                 | i     | A                         |

The SOFC stack simulated in this paper consists of 30 single cells with a current of 43 A, a voltage of 30 V and a power of 1290 W. The SOFC voltammetric characteristic curve obtained through simulation is shown in Figure 2 below.
Fig. 2 Volt-ampere characteristic curve of SOFC

A The SOFC volt-ampere characteristic curves obtained from simulation and experiment are shown in Figure 2, where the maximum error between the simulation results and the experimental results is 3%. This shows the correctness of the simulation model.

The variation of the stack output voltage versus the air inlet pressure when the other input parameters are held constant and only the air inlet pressure is varied is shown in Figure 3.

Fig. 3 Stack voltage curve at different air inlet pressure

As shown in Figure 3, the output voltage of the stack gradually increases as the air inlet pressure gradually increases, but tends to slow down. This is because the increase in air inlet pressure causes the ideal reversible voltage $E$ of the stack to gradually increase, while the cathode activation polarization $\eta_{act,c}$ gradually decreases, thus gradually increasing the output voltage of the stack.

The relationship between stack output efficiency and air inlet pressure is shown in Figure 4.
As can be seen from the graph, the output efficiency of the reactor gradually increases as the output current of the reactor increases, and when the air inlet pressure gradually increases, the output efficiency of the reactor also gradually increases, and the maximum increase in the efficiency of the reactor can be 4%, but the increase is gradually decreasing.

A comparison of the effect of fuel inlet pressure on stack output voltage and the effect of air inlet pressure on stack output pressure is shown in Figure 5 below.

It is clear from Figure 4 that the effect of air inlet pressure on stack performance is greater than the effect of fuel inlet pressure on stack performance. The maximum increase in stack output voltage is 1.1% when the fuel inlet pressure is increased, and 3.1% when the air inlet pressure is increased.

When the fuel inlet pressure and air inlet pressure are increased simultaneously, the effect on the stack performance is shown in Figure 5.
As can be seen from the above graph, when the SOFC bipolar inlet pressure is increased at the same time, the output voltage of the reactor increases significantly, while it is much higher than the output voltage of the reactor when the fuel inlet pressure is increased, compared to the atmospheric pressure case, when the bipolar inlet pressure is increased at the same time, the output voltage of the reactor can be increased by a maximum of 4.9%.

When the cathode inlet gas flow rate is kept constant and the percentage of nitrogen and oxygen is changed, the output power of the SOFC system changes as shown in Figure 6.

As can be seen in Figure 7, as the percentage of oxygen increases, the SOFC output power also gradually increases, and the higher the input current, the more obvious the effect of oxygen content on the output performance of the stack. When the percentage of nitrogen and oxygen is 1:1, the output power of the reactor can be increased by a maximum of 4.5% compared to air, and when the input is pure oxygen, the output power of the reactor can be increased by a maximum of 6.7% compared to air.

4. Conclusion
Through modelling simulation analysis and reference to experimental data, the following conclusions are obtained.

The SOFC model built in this paper based on Matlab/Simulink is correct.

Increasing the air inlet pressure can effectively improve the output voltage and efficiency of the stack, with a more obvious effect, the output voltage can be increased by a maximum of 4%.
When the air inlet pressure of both poles is increased simultaneously, the output performance of the stack can be significantly improved, and the output voltage can be increased by a maximum of 4.9%. For the existing 1KW SOFC reactor in the laboratory, it is most appropriate to increase the fuel electrode to 2 times the atmospheric pressure, because the increase in pressure will lead to an increase in temperature, and a too high temperature will cause damage to the reactor.

The cathode inlet gas flow rate remains constant and the output power of the SOFC gradually increases as the percentage of oxygen increases. When the percentage of nitrogen and oxygen is 0:1, the maximum power output of the stack can be increased by 6.7%.

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