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Numerical simulation of solid oxide fuel cell with multi-physical coupling

Zihao CHEN
College of Pipeline and Civil Engineering, China University of Petroleum, Shandong, China

Abstract
The numerical model of solid oxide fuel cell (SOFC)with multi-physical coupling is established, and the model of SOFC was calculated by finite element method. The electrochemical performance of SOFC using H_2 as fuel is studied bythis method. The results show that the power density of SOFC increases first and then decreases with the increase of current density. And the power density reaches the maximum when the current density is 5457 $A{\cdot}m^{-2}$.The highest temperature of SOFC is 938 ℃, the lowest temperature is 815 ℃, and the temperature difference is 123 ℃ The utilization rate of H_2 is 44.5%.
Keywords: *solid oxide fuel cell,multi-physical coupling, electrochemistry, temperature.*

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I. INTRODUCTION

Solid oxide fuel cell (SOFC) is a kind of energy source installation which can convert chemical energy into electric energy directly[1]. It has the advantages of high rate of energy conversion, low noise and wide applicabilityof fuel[2].The operating temperature of SOFC is 600~100 degrees. The materials of SOFC under the condition of high temperature show creep phenomenon and produce thermal stress, which will affect the mechanical life of the structure.Suwanwarangkul et al.[3] established a 1-D steady-state model of SOFC and assumed that the current density was uniformly distributed at the interface of electrolyte and anode to study the transfer of gas components. Jeon et al. [4]established a SOFC hydrodynamics model based on the coupling of gas flow and heat transfer.

SOFC experiment has the disadvantages of high cost, long cycle and low success rate. And the operating condition of the SOFC is close state, so some physical quantities are difficult to measure. Numerical simulation can clearly show the distribution laws of various physical quantities.Numerical simulation can clearly show the distribution law of various physical quantities steady state condition, including current density, gas concentration and temperature of SOFC. Therefore, numerical simulation becomes an important method to study SOFC.

II. MODELING

In the process of modeling, it is necessary to simplify the model reasonably in order to reduce the calculation difficulty and improve the applicability of the model without affecting the calculation results.

i. The gases in the SOFC is considered as ideal gases;
ii. The mode of fluid flow is considered as advection;
iii. The running state of SOFC is steady;
iv. H_2O in the anode is not used as reactant.

2.1 Model of geometry

The structure of the planar solid oxide fuel cell is composed of metal connectors, anode, electrolyte, cathode and anode support. The geometric model of the single-channel SOFC used in this paper is shown in the Fig 1.

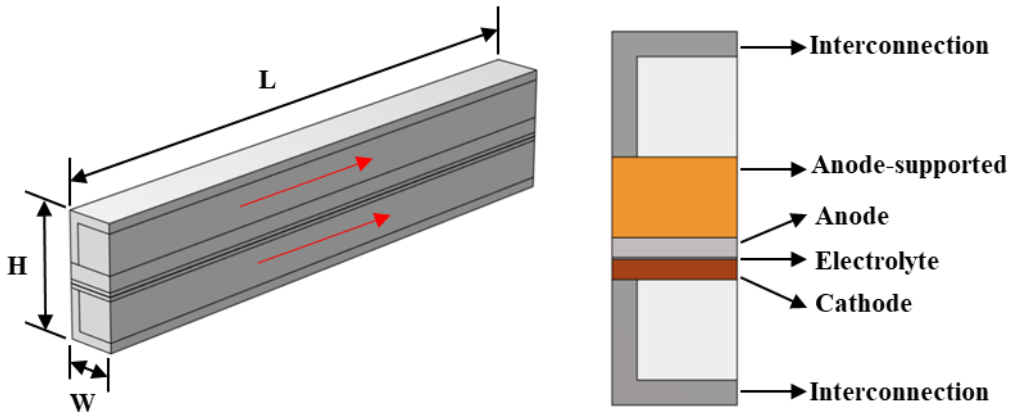

Fig. 1: Model of the single SOFC

Since the L of SOFC is much larger than the directions of H and W, the length direction is displayed in a proportion of 0.1 for the convenience to observe.The red arrow in the Fig.1 shows the direction of gases flow.

2.2 Mathematical modelling

2.2.1 Electrochemical model

In SOFC, H_2 is oxidized in the anode and O_2 is reduced in the cathode. The equations are as follows:

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \tag{1.1}$$

$$O_2 + 4e^{2-} \rightarrow 2O^{2-} \tag{1.2}$$

The Butler-Volmerequation [5]is used as the governing equation to calculate the current density:

$$i_{\text{loc}} = i_{0,\text{ref}} \left(\sum_{\text{i:}v_i>0} \left(\frac{a_i}{a_{i,\text{ref}}}\right)^{v_i} \exp\left(\frac{\alpha_a F \eta_{\text{ref}}}{RT}\right) - \sum_{\text{i:}v_i>0} \left(\frac{a_i}{a_{i,\text{ref}}}\right)^{-v_i} \exp\left(\frac{-\alpha_c F \eta_{\text{ref}}}{RT}\right)\right) \tag{1.3}$$

where α is transfer coefficient, i_0 is the exchange current density of reference, η is the electric potential, F is Faraday constant, R is the ideal gas constant, T is temperature, a is molar concentration of gas, v_i is reaction coefficient.

2.2.2 Diffusion model

The diffusion of gases follows the mass conservation equation[6]. AndMaxwell-Stefan equation is used for calculation:

$$\nabla \cdot (\rho \omega_i u) = -\nabla \cdot \left(-\rho \omega_i \sum_{k=1}^{Q} D_{ik} d_k - D_i^T \nabla \ln T\right) + R_i \tag{1.4}$$

whereρ is the density of the mixed gases, ω_i is the mass fraction of gas-i, $u$is the average velocity of the mixture, R_i is the change rate of the material source, Q is the number of types of gases, D_{ik} is the coefficient of Fick diffusion, d_k is the force of diffusion driving applied to material k,D_{iT} is the coefficient of thermal diffusion.

2.2.3 Flow model

Navier-Stokes equations[7] and Brinkman equations are used as the governing equations for gas flow:

$$\nabla \cdot (\rho u) = Q_m \tag{1.5}$$

$$\rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nabla \cdot [-p\boldsymbol{I} + \boldsymbol{\tau}] + \boldsymbol{F} \tag{1.6}$$

$$\frac{\rho}{\varepsilon_p}\left((\boldsymbol{u} \cdot \nabla)\frac{\boldsymbol{u}}{\varepsilon_p}\right) = -\nabla p - \left(\kappa^{-1}\mu + \frac{Q_m}{\varepsilon_p^2}\right)\boldsymbol{u} + \boldsymbol{F} + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T) - \frac{2}{3}\mu(\nabla \cdot \boldsymbol{u})\boldsymbol{I}\right\}\right] \tag{1.7}$$

where$\boldsymbol{u}$ is the velocity vector, p is the pressure, $\boldsymbol{I}$ is the unit tensor, $\boldsymbol{\tau}$ is the viscous stress tensor, $\boldsymbol{F}$ is the volume force tensor, ε_p is the porosity of the porous medium, μ is the dynamic viscosity, κ is the permeability of the porous medium.

2.2.4 Heat transfer model

The heat sources of SOFC are mainly electrochemical heat and ohm-heat. The transfer of heat between various structures is:

$$\rho C_p u \cdot \nabla T + \nabla \cdot (-k \nabla T) = Q \tag{1.8}$$

whereC_p is the heat capacity at constant pressure, Q is the source of heat, and k is the thermal conductivity.

2.3 Boundary conditions

The operating voltage of SOFC is 0.7V. The operating temperature and gas temperature are 800 ℃.The working pressure is 1 atm. The flow velocity at the entrance of air is 1.0 m/s, and the flow velocity at the entrance of fuel is 0.5 m/s.

The composition of air and fuel is shown in Table 1.

Table 1: The component of gases (wt. %)

Type of gas	O_2	N_2	H_2O	H_2
Air	0.21	0.79	—	—
Fuel	—	0.2	0.4	0.4

III. RESULT AND DISCUSSION

3.1 Electrochemical performance

Fig.2 is the curves of current density and power density calculated by the multi-physics coupling numerical model under this working condition. It can be seen from the Fig. 2 that the voltage decreases with the increase of the current density. The power density increases first and then decreases with the increase of current density. When the current density is5457A·m^{-2}, the maximum power density is 2728.5W·m^{-2}.

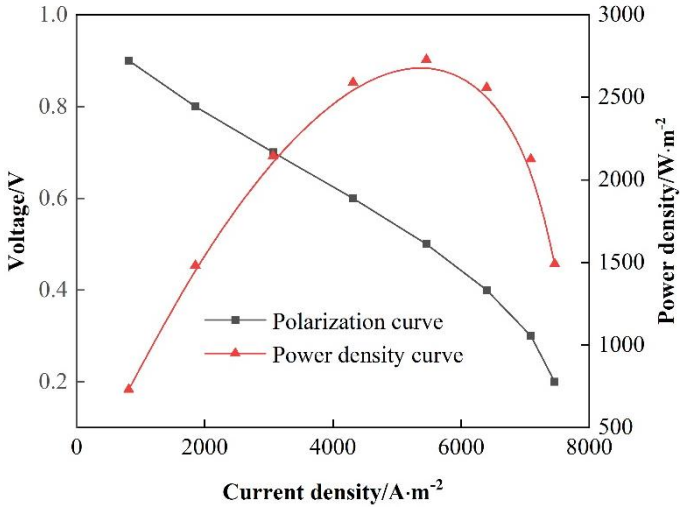

Fig. 2: Electrochemical performances

Fig. 3 is the current density distribution on the electrolyte when the operating voltage is 0.7 V. It can be seen from Fig. 3 that the maximum current density is 3220A·m^{-2}at the entranceof the channel. The minimum current density is 2920 A·m^{-2} at the exit. The general distribution trend of current density decreases gradually along the direction of gas flow. The reason is that the concentration of H_2 and O_2 at the entrance of the channel is the largest. And the rate of electrochemical reaction is the largest, so the current density is the largest. With the consumption of gases, the rate gradually decreases and the current density decreases.

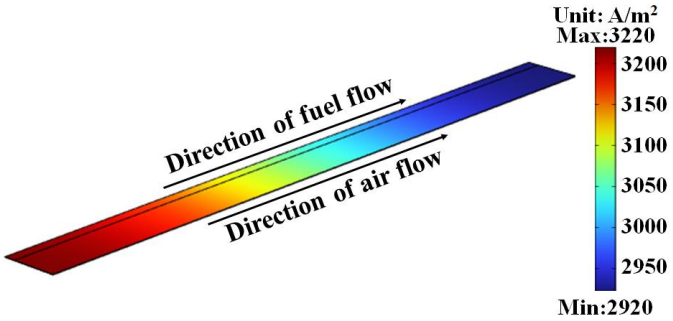

Fig. 3:Distribution of electric current density on the electrolyte

3.2 Distribution of temperature

In SOFC, the electrochemical reaction will generate heat and the transfer of current will generate ohm-heat.So the overall temperature of SOFC is rising. It can be seen from the Fig.4, when the operating voltage is 0.7V, the lowest temperature is 815℃at the entrance of gases, while the highest temperature is938℃at the exit of gases. The overall distribution of temperature is that the temperature increases gradually along the direction of gases flow. With the progress of electrochemical reaction, the heat increases continuously, and the temperature at the entrance of the gases is low and the specific heat capacity of the air is large, which has the cooling effect for SOFC. As the gas flows, heat accumulates and reaches its maximum temperature at the exit of

gases.

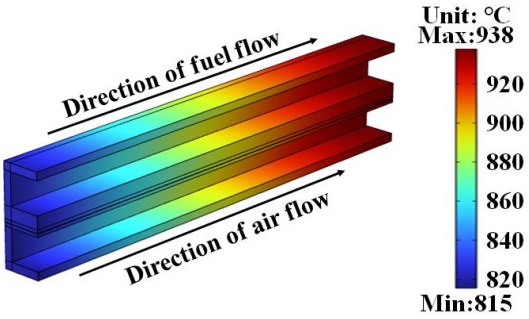

Fig. 4: Temperature distribution of the SOFC

3.3 Distribution of gas components

Fig. 5 shows the distribution of the molar concentration of H_2 in the fuel channel, anode support layer and porous anode at the operating voltage of 0.7 V. It can be seen from Fig. 5 that the molar concentration of H_2 decreases along the direction of gases flow. The maximum value is 9.75 mol/m^3 at theentrance of fuel and the minimum value is 5.41 mol/m^3 at the exit of fuel. The main reason is that with the electrochemical reaction, H_2 is consumed continuously and H_2O is generated at the same time, which leads to the continuous decrease of H_2 concentration.The utilization rate of H_2 is about 44.5%.

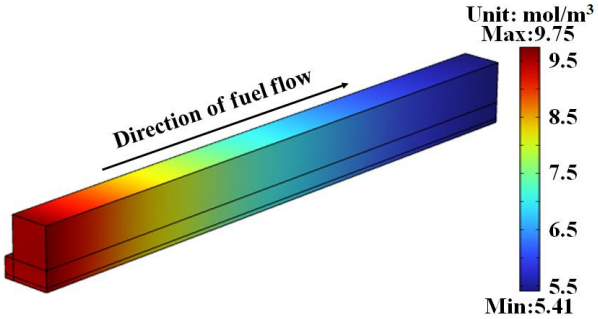

Fig. 5: Distribution of molar concentrations of H_2

IV. CONCLUSION

A single channel SOFC numerical model with multi-physical coupling is established, and the model of SOFC using H_2 as fuel was calculated by finite element method. The electrochemical performance, temperature distribution and gases component distribution of SOFC are studied. The specific law is as follows:

i. The current density decreases with the increase of operating voltage. With the increase of current density, the power density first increases and then decreases. When the current density is 5457 A·m^{-2}, the maximum power density is 2728.5 W·m^{-2}.

ii. The current density on the electrolyte decreases along the direction of gases flow. The maximum value is 3220 A·m^{-2} and the minimum value is 2920 A·m^{-2}.

iii. The temperature of SOFC increases along the direction of gases flow. The maximum value is 938 ℃and the minimum value is 815 ℃.

iv. The concentration of H_2 decreases along the direction of gases flow, and the utilization rate of H_2 is 44.5%.

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