Structure optimization and thermal field analysis of biogas derived methane fueled Solid Oxide Fuel Cell

Ruobing Zhan, Yang Wang, Qing Du* and Kui Jiao*
State Key Laboratory of Engines, Tianjin University, Tianjin, 300350, China
*Corresponding author’s e-mail: kjiao@tju.edu.cn (K. Jiao); duqing@tju.edu.cn (Q. Du)

Abstract. The suitability for using various gaseous fuels makes the Solid Oxide Fuel Cell (SOFC) the most promising heat-electricity cogeneration device. Thermal field distribution of SOFC directly determines whether the cell is operating in sufficient catalytic activity and weakened by thermal stress. For biogas derived methane fueled SOFC, the internal reforming reactions can cause the inhomogeneous temperature distribution. So it is crucial to optimize the thermal field to achieve optimal cell operation state. In this paper, a 3D multi-physics model is developed to study the improvements of a new cathode flow field structure. When adopting new cathode structure, the power density increases by over 11%, and the maximum temperature gradient can be evidently reduced.

1. Introduction
Among many energy conversion devices, Solid Oxide Fuel Cell (SOFC) possesses an excellent fuel flexibility, which can be fueled by H₂, coal syngas and various alcohol fuels [1]. Besides, after purification and upgrading, the biogas can be refined as high purity methane which is a non-polluting high heating value fuel. For methane fueled SOFC, the cell thermal management is mainly carried out by adjusting the cathode air flow rates. The temperature distribution and the maximum temperature gradient must be controlled within a reasonable range which insures a high catalyst activity without excessive thermal stress [2].

There are many studies on the flow field optimization [3-5]. Among them, Wei et al. [6] replaced the cathode flow channel as a porous cathode current collector, and the relevant simulations are performed. Zielke et al. [7] employed a Cu-Mn alloy made metal foam as the cathode contact material to enhance the conductivity of cathode electrode. The experimental results show that this new type of cathode structure can significantly improve the cell output performance, and the endurance of this new structure against long-time oxidation is verified.

In this study, inspired by Zielke’s experiment, an optimized cathode structure of SOFC is presented. And the cell performance and thermal field analysis are conducted by developing a 3D multi-physics SOFC model. Compared to traditional straight channel flow field, the improvements of optimized structure are discussed in detail.

2. Modeling development

2.1 Cell geometry
The anode-supported planar SOFC are adopted in this study. For typical anode-supported SOFC, the cell is consist of interconnects, anode/cathode channels and the positive electrode-electrolyte-negative
electrode (PEN). The partly pre-reformed methane is supplied as the fuel to the anode inlet. And the chemical and electrochemical reactions proceeds inside the porous electrode inside PEN. The cell geometries of two kinds of flow fields are shown in Figure 1. For the new cathode structure, different from the straight channel flow field, the porous media (normally metal foam) is placed in the position between cathode interconnect and PEN as the air channel.

2.2 Governing equation
The heat and mass transfer, fluid flow and the chemical/electrochemical reactions are highly coupled in present model. And the conservation equations are listed in Table 1. The multi-component diffusion process (molecular diffusion and Knudsen diffusion) are considered in this model. The effective multi-component diffusion coefficients \( D_{\text{eff}} \) and the related source terms \( S \) can be found in Ref [8].

| Description          | Conservation Equations                                                                 |
|----------------------|----------------------------------------------------------------------------------------|
| Mass                 | \( \frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho \phi \mathbf{v}) = S_m \) |
| Momentum             | \( \frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\rho \mathbf{v} \cdot \nabla \rho + \nabla \cdot \left[ \mu \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) \right] + S_u \) |
| Species              | \( \frac{\partial (\rho_i \phi_i)}{\partial t} + \nabla \cdot \left( \rho_i \mathbf{v} \phi_i + \rho_i \mathbf{v} \nabla \phi_i \right) = S_i \) |
| Energy               | \( \frac{\partial (\rho \phi_T)}{\partial t} + \nabla \cdot (\rho \mathbf{v} \phi_T) = \nabla \cdot (\kappa \nabla T) + S_e \) |
| Electronic charge    | \( 0 = \nabla \cdot (\sigma_{\text{ele}} \nabla \phi_{\text{ele}}) + S_{\text{ele}} \) |
| Ionic charge         | \( 0 = \nabla \cdot (\sigma_{\text{ele}} \nabla \phi_{\text{ele}}) + S_{\text{ele}} \) |

2.3 Chemical and electrochemical model
When the methane contained gas is supplied to SOFC, several internal reforming reactions occurs simultaneously. Thereinto the methane steam reforming reaction (MSR) and the water gas shift reaction (WGSR) play a leading role, and can be described by following reactions:

\[
\text{MSR:} \quad \text{CH}_4 + \text{H}_2\text{O} \leftrightarrow \text{CO} + 3\text{H}_2 \tag{1}
\]

\[
\text{WGSR:} \quad \text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \tag{2}
\]

The strongly endothermic reaction, MSR, will have an impact on the cell temperature gradient distribution. Thus, in this study, these two reactions are both considered with the same reaction rate.
expressions as Haberman’s model [9]. The related equations (reaction rates and reaction heats) can be found in our previous study [8].

The cell output voltage is calculated as the following expression:

\[ V_{\text{output}} = E_{\text{rev}} - \eta_{\text{act}} - \eta_{\text{ohm}} \]  \hspace{1cm} (3)

where the reversible voltage \( E_{\text{rev}} \) can be obtained as:

\[ E_{\text{rev}} = -\frac{\Delta G^0}{2F} + \frac{RT}{2F} \ln \frac{p_{H_2,CO} P_0^{0.5} p_0^{-0.5}}{p_{H_2,O,CO_2}} \]  \hspace{1cm} (4)

We take account of the coupled \( H_2/CO \) electrochemical oxidation which is assumed to occur in anode catalyst layer. The expressions of anode and cathode electrochemical reaction rates (\( J_a \) and \( J_c \)) are determined by the Butler-Volmer equations:

\[ J_a = J_0 a \frac{A_v}{A} \left[ \exp \left( \frac{\alpha 2F \eta_{\text{act,a}}}{RT} \right) - \exp \left( -\left(1 - \alpha \right) \frac{2F \eta_{\text{act,a}}}{RT} \right) \right] \]  \hspace{1cm} (5)

\[ J_c = J_0 c \frac{A_v}{A} \left[ \exp \left( \beta \frac{4F \eta_{\text{act,c}}}{RT} \right) - \exp \left( -\left(1 - \beta \right) \frac{4F \eta_{\text{act,c}}}{RT} \right) \right] \]  \hspace{1cm} (6)

where \( A \) is the electrochemical active area (\( m^2 \)), \( J_0 \) the exchange current density (A \( m^{-2} \)), \( \alpha \) and \( \beta \) the transfer coefficient, \( \eta_{\text{act}} \) the activation overpotential (V). It should be mentioned that the exchange current density of CO is supposed to be 1/3 of that of \( H_2 \) due to the CO’s low catalyst activation.

2.4 Numerical procedures

The commercial software Fluent solver is employed to solve the conservation equations. And the in-house C code are compiled as the user defined functions (UDF) to simulate the multi-component diffusion process and the chemical/electrochemical reactions. Besides, the mesh-independence tests are carefully conducted to guarantee the error caused by mesh is in allowable range.

3. Results and discussions

3.1 Experimental comparison

The experiment validation is conducted in different operating temperature. The operating conditions and cell parameters are consistent with the experiment [10]. In order to validate the coupled electrochemical oxidation effects of \( H_2 \) and \( CO \), two kinds of fuels (pure \( H_2 \) and coal derived syngas) are selected, and the C-V curves are shown in Figure 2, in which the simulation results fit the experiment data well.

![Figure 2. Experimental comparison: (a) pure \( H_2 \) (b) Syngas.](image_url)
3.2 Structure optimization

In order to investigate the effects of new cathode structure, a six-channel single cell and the corresponding single cell with the porous material flow field are simulated. The Current-Voltage (C-V) curves and Power-Voltage (P-V) curves of two kinds of cells are shown in Figure 3. As the results shown, the new cathode structure can significantly improve the cell output performance, and the increment can reach to over 11%. Figure 4 shows the electrochemical reaction rates at the interface of cathode catalyst layer (CL) and electrolyte (ELE). For straight channel flow field, there are some oxygen-deficient areas which will result in zero reaction rates. In contrast, the new cathode structure can make the reaction rates concentrate on a small range. The same tendency can be found in the species distribution field. Besides, the porous material flow field completely contacts with the porous electrode, which markedly decreases the contact resistance. All these factors contribute to improve the cell output performance.

![Figure 3. C-V and C-P curves comparisons.](image1)

![Figure 4. Electrochemical reaction rates at the interface of CL/ELE.](image2)

3.3 Thermal analysis

For SOFC, the extra heat is mainly taken away by the air. It should be mentioned that the air amount supplied to cathode inlet remains unchanged for all cases. When the fuel concluding methane is fed in the cell anode, the MSR mainly proceeds in front of the cell. In some cases, this endothermic reaction may make the cell inlet temperature less than the inlet gas temperature. But as the heat accumulates along the flow direction, the temperature of the end of the cell is raised greatly. For these reasons, the temperature gradient is normally large.

Figure 5 shows the temperature distribution of two structures. The maximum temperature gradient of the optimized flow field is 105K which is much less than the traditional one. Table 2 lists each heat source terms of two structures. It is observed that the main difference lies in the ohmic heat. As mentioned above, the porous material flow field can sufficiently contact with the cathode porous electrode, which means that this structure can break through the limitation of the channel-rib structure of straight channel. The electrons are directly transfer to the interconnect through the porous material without the horizontal transfer process inside porous electrode. This process can decrease the electron transfer distance, and reduces the ohmic loss. Then, the ohmic heat is reduced.
4. Conclusions
We developed a multi-physics biogas derived methane fueled SOFC model to investigate the effects of the optimized cathode structure on the cell performance. Compared with the straight-channel cell, the cell adopting the porous material flow field shows a larger output voltage. Meanwhile, the distribution of the electrochemical reactions gets more uniform and concentrates within a small range. Besides, through the contrastive study on the heat source terms, we found the main influence factor on the maximum temperature gradient is the ohmic loss. And the sufficient connection between porous material flow field and porous electrode reduces the contact resistance. The total extra heat production of the optimized structure decreases of almost 20%. The maximum temperature gradient drops by 32K.

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