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Numerical analysis of optimal performance of planar electrode supported solid oxide fuel cell at various syngas flow rates

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ABSTRACT

With the gradual scarcity of fossil fuels and the emergency demand of greenhouse gas emission reduction, coal, as the major energy source of China for a long time in the future, should be used efficiently and cleanly. The integrated gasification fuel cell (IGFC) hybrid power generation system is a promising clean coal utilization technology. In order to improve the performance of IGFC hybrid power generation system, the optimal performance of SOFC at different flow rate of syngas were numerically studied in this work. The performance curves of SOFC at various syngas flow rates were obtained. The results show that the temperature in the channel of SOFC cell is decreasing linearly with the increase of the syngas flow rate, when the average current density is constant. With the increase of syngas flow rate, the output voltage is reduced, but the optimal output power and the possible optional range of current density will increase. Under different mass flow rates, the fuel utilization at the optimal output power density decreases with increase of syngas flow rate. The polynomial function between the fuel utilization at optimal output power density and the mass flow rate of syngas was obtained.

1. Introduction

Since alternative energy sources are not sufficient to cover the great increasing primary energy demand in China, coal, as the most abundant fossil fuel with the most evenly distributed reserves, is expected to be the future key fuel [1,2]. The conventional methods of using coal have many disadvantages such as low-efficiency, high-emission and so on. The technology of integrated gasification fuel cell (IGFC) hybrid power generation system makes up these shortcomings with the efficient and clean utilization of coal. Coal syngas could be applied as a fuel for a combined-cycle power plant with coal gasifier, SOFC, and gas/steam turbines [3,4]. Among these plants, SOFC offers significant advantages compared to other types of fuel cells, such as the capability of internal reforming or even direct oxidation of carbon-based fuels, environmental compatibility (low NOx production), high fuel-to-electricity conversion efficiency, modularity and no need for higher cost precious metal catalyst [5–7].

Based on the characters of SOFC and coal, the operation of solid oxide fuel cells using different types of carbon-based fuels (i.e. natural gas, coal syngas, etc.) became one of the main topics of SOFC research in the past few years. The main compositions of coal syngas are carbon monoxide, hydrogen, carbon dioxide, steam and methane, as well as impurity and trace species. Andre Weber et al. [8] investigated oxidation of H_2, CO and methane in SOFCs with Ni/YSZ-cermet anodes. As the research showed, in the case of CO/H_2 mixtures, the increasing CO was bad for the performance of SOFC especially when CO portion is higher than 90%, whereas the cell performance increased with decreasing S/C ratio fueled with methane. In addition, the stability of single cells was investigated. The cell operated stably for 1000 h without serious degradation using dry methane as fuel (S/C = 0). Alzate-Restrepo and Hill [9] researched carbon deposition on Ni/YSZ anodes using CO/H_2 as fuel under the working conditions of temperature at 1073 K and open circuit potential or with a current density of 10 mA cm^{-2}. It is known from the results that the polarization resistance increased because of carbon formation and the anodes deactivated. In the worst case, an anode delaminated after 6 h of operation using 75–25% CO/H_2 at OCP. In the best case, an anode had stable performance with no carbon formation for over 6 h using pure CO at a current density of 10 mA cm^{-2}.

Because the output power of IGFC system depends on the users' demands which change over time, it is necessary to investigate the off-design performance of SOFC stack in detail. However, it is very difficult and expensive to study the off-design performance of SOFC stack by experiments in all operating states. Therefore, in this work, the optimal performances of SOFC under different syngas flow rates were studied based on the numerical analysis. In our

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Nomenclature

A_i	pre-exponential factor
C_e	effective factor
F	Faraday's constant: 96,487 (C mol^{-1})
$E_{a,i}$	activation energy (J kmol^{-1})
E_{TPB}	electromotive force (V)
ΔG^0	Gibb's free energy change under standard states (J kg^{-1})
$\Delta H^0_{298.15}$	heat of reaction (J kmol^{-1})
ΔH^0_i	heat of chemisorption (J kmol^{-1})
H_{fuel}	enthalpy of fuel (J kg^{-1})
j_{ave}	average current density (A m^{-2})
$K_{eq,i}$	equilibrium constant
k_i	reaction rate constant
κ_i	adsorption constant of component i
m	mass flow rate (10^{-6} kg s^{-1})
P_i	partial pressure of component i (kPa)
P_{den}	output power density (W m^{-2})
R	universal gas constant (J kg^{-1} K^{-1})
r_i	reaction rate (kmol h^{-1} kg cat^{-1})
T	temperature (K)
V_{out}	output voltage (V)

Greek symbols

η_{fuel}	fuel utilization
η^{act}	over-potential incurred by activation polarization (V)
η^{ohm}	over-potential incurred by ohmic resistance (V)

previous work, the novel structures of planar SOFC and the materials of electrodes and electrolyte were developed, and the 3D computational models were validated by the experiment using hydrogen and methane as fuel [10–13]. Also, the optimization and simulation of gasifier for poly-generation system was conducted [14]. Comparing with the previous models of SOFC, the fully three-dimensional models were used in this work. The coupled heat transfer of solid and fluid in porous media was considered as well. Moreover, the validated data of heat transfer, diffusion and viscidity was obtained from the experiments and literature [10]. In addition, the gas diffusion in porous media was taken into account instead of the simple empirical formula used to calculate the over-potential of concentration. Furthermore, the effective kinetic models obtained from experiments [13] were used to analyze the relating chemical reaction models in this work. On the basis of previous work, fully 3D mathematical models for planar SOFC cell using syngas were built based on commercial CFD software (CFX4.4). The optimal performance of SOFC with the developed materials and structures were investigated under different mass flow rates of syngas. These results are expected to be helpful to develop the IGFC system.

2. Computational models

In SOFC stacks, most of single cells in a stack almost work at the same conditions for the series connection structure. The performance of single cell can indicate the performance of SOFC stack. In a SOFC cell, heat and mass transfer are coupled with each other, and these physical processes are controlled by 3D N–S equations. Though the laminar flow mainly occurs in porous media, the turbulent flow in gas passages, especially in air flow passages, should be considered. The effect of turbulence is represented by the $k-\varepsilon$ model. In the porous media, the porosity and permeability should be considered. Thus, both Navier–Stokes equations and Darcy's law are used in the model of heat/mass transfer. Meanwhile, molecular diffusion and Knudsen diffusion in mass transfer process are considered as well [15,16]. In addition, the effective thermal conductivity of porous media can be obtained from the volume averaged conductivity of fluid and solid.

2.1. Electrochemical models

By electrochemical model, electric potential, current and output power can be calculated. The electromotive force is determined by a well-known Nernst equation which is yielded by the oxidation of H_2 and depends on the gas composition and temperature.

$$E_{TPB} = \frac{-\Delta G^{\circ}}{2F} + \frac{RT}{2F}\ln\left(\frac{P_{H2,TPB}P^{0.5}_{02,TPB}}{P_{H2O,TPB}}\right) \quad (1)$$

In the above equation, the partial pressure of each gas component is its partial pressure at the three-phase interface. Therefore, the over-potential of concentration is considered in the above equation. In this work, the activation over-potential (η^{act}) is calculated by the non-linear Butler–Volmer equation, which is controlled by the electrode kinetics at the electrode surfaces [17]. Thus, the output voltage can be obtained as follow.

$$V_{out} = E_{TPB} - \eta^{act} - \eta^{ohm} \quad (2)$$

For SOFC, the output power density, fuel utilization and energy efficiency are important parameters to evaluate its performance. In this work, the output power density P_{den} is given by:

$$P_{den} = V_{out} \times j_{ave} \quad (3)$$

The fuel utilization η_{fuel} is given by:

$$\eta_{fuel} = \frac{H_{fuelin}H_{fuelout}}{H_{fuelin}} \quad (4)$$

2.2. Chemical reactions in anode

The syngas from coal gasification mainly consist of H_2, CO, H_2O, CO_2 and CH_4, and is supplied to the anode. In this work, the composition of syngas from Texaco/Illinois 6 gasifier is listed in Table 1 [14,18]. Due to the complexity of syngas components, the overall chemical reactions in anode are listed in Ref. [13] in detail. Generally, when pure CO is supplied, oxidized CO must be considered in an electrochemical reaction at the anode. When the shift reaction is available, its reaction rate is very fast at high temperature [19].

Table 1
Composition of syngas.

Composition	Molar fraction (%)
CO	39.58
H_2	30.28
CO_2	10.78
H_2O	16.45
CH_4	0.079
N_2	2.831