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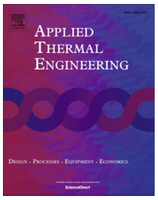

Research Paper

The thermal effect in direct carbon solid oxide fuel cells

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HIGHLIGHTS

- A model for the thermal effect in DC-SOFC is developed.
- Operating parameters greatly influences the DC-SOFC thermal behaviors.
- The temperature field in DC-SOFC is highly non-uniform.
- A breakdown of heat generation/consumption in DC-SOFC is given.

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ABSTRACT

In this paper, the thermal effect in a tubular direct carbon solid oxide fuel cell (DC-SOFC) is studied with a numerical model. After model validation, parametric simulations are carried out to study the effects of operating and structural parameters on the thermal behaviors of DC-SOFCs. It is found that the thermal behaviors of DC-SOFC greatly depends on operating parameters and the temperature field in DC-SOFC is highly non-uniform. The position of peak temperature in the cell is highly dependent on the operating potential. In addition, a smaller distance between the carbon bed and the anode is beneficial for improving the temperature uniformity in the DC-SOFC. The breakdown of heat generation/consumption in DC-SOFC shows that the anode processes contribute the most to the temperature variation in the cell. The results of this study form a solid foundation for better thermal management of DC-SOFC.

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1. Introduction

Solid carbon can be obtained easily from fossil fuels or cheap and renewable biomasses such as wood and leaves. Solid carbon fuels are usually used for power generation by conventional heat engines which will emit significant amount of various pollutants (i.e. SO_x, CO_2, and NO_x) as byproduct [1,2]. Besides, the efficiency of conventional thermal power plant is typically below 40% or even about 30% if carbon capture and storage is adopted to reduce the pollutant emission [3]. Although relatively new gas fired CCGT thermal power plant and coal fired power plant have reached an efficiency of 55% and 40%, respectively [4], more efficient and environmental friendly strategy using solid carbon fuel for power generation is still of practical importance as solid carbon will be used for energy conversion for a long time.

Solid oxide fuel cell (SOFC) is an advanced energy conversion device converting the fuel into electricity through electrochemical reaction with a high efficiency (50–60%) [5,6]. An SOFC has an all solid-state structure with a dense electrolyte placed between the porous anode and cathode. In SOFCs, the fuel and oxygen are separated by the oxygen-ion-conducting membrane, resulting in easy pollutant control. The high temperature of SOFCs (i.e. 800 °C) facilitates the electrochemical reaction kinetics and low cost catalyst (i.e. Nickel) can be used. SOFCs are fuel flexible. Various alternative fuels, such as H_2, various hydrocarbons, NH_3 and even solid carbon can be used in SOFC for electricity generation [7,8].

The direct use of solid carbon as a fuel in SOFCs offers a new strategy for efficient power generation with low environmental impact. The direct-carbon solid oxide fuel cell (DC-SOFC) has received extensive research since Nakagawa and Ishida [9] first prepared and tested DC-SOFCs. They also proposed the "CO_2 shuttling theory" as the working mechanisms of DCFC. It's proposed that the reaction between carbon and CO_2 produces CO, which is electrochemically oxidized at the DCFC anode. Lee et al. [10]

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Nomenclature

Abbreviations

DC-SOFC	solid oxide fuel cell direct using carbon as fuel
PEN	positive electrode-electrolyte-negative electrode assembly
SCCM	standard cubic centime per minute
SOFC	solid oxide fuel cell
TPB	triple phase boundary

Roman

B_0	permeability coefficient, m^2
c_{CO_2}	molar concentration of carbon dioxide, mol m^{-3}
C_p	heat capacity, J K^{-1}
D_{ce}	distance between carbon and anode
D_i^{eff}	effective diffusivity of species *i*, $m^2\ s^{-1}$
D_{ik}^{eff}	Knudsen diffusion coefficient of *i*, $m^2\ s^{-1}$
D_{im}^{eff}	molecular diffusion coefficient of *i*, $m^2\ s^{-1}$
E_a	active energy, J mol^{-1}
E_{CO}	equilibrium potential for carbon monoxide oxidization, V
E_{CO}^0	standard equilibrium potential for carbon monoxide oxidization, V
E_{eq}	equilibrium Nernst potential, V
E_{rb}	active energy of Boudouard reaction, J mol^{-1}
F	Faraday constant, 96,485 C mol^{-1}
i_o	exchange current density, A m^{-2}
k_{rb}	equilibrium constant of Boudouard reaction, s^{-1}
L_{cell}	length of the cell, mm
n	number of electrons transferred per electrochemical reaction
N_i	flux of mass transport, kg $m^{-3}\ s^{-1}$
p	(partial) pressure, Pa
R	gas constant, 8.314 J $mol^{-1}\ K^{-1}$
R_{ce}	ratio D_{ce} and cell length
R_{ce}	reaction rate of Boudouard reaction, mol $m^{-3}\ s^{-1}$
T	temperature, K
u	velocity field, $m^3\ s^{-1}$
V	volume fraction
y_i	molar fraction of component i

Greek letters

α	charge transfer coefficient
β_{H_2}	electrochemical kinetics parameter for H_2
ε	porosity
$\eta_{act,an}$	anode activation polarization, V
$\eta_{act,ca}$	cathode activation polarization, V
η_{ohmic}	ohmic polarization, V
κ	permeability, m^2
λ	thermal conductivity, W $m^{-1}\ K^{-1}$
μ	dynamic viscosity of fluid, Pa s
ρ	fluid density, kg m^{-3}
σ	conductivity, S/m
τ	tortuosity
$\varnothing$	potential, V

Subscripts

an	anode
ca	cathode
co	carbon monoxide
l	ionic phase
s	electronic phase

Superscripts

0	parameter at equilibrium conditions
eff	effective
L	local

performed system exergy analyses of DC-SOFCs and found that the DC-SOFCs were more efficient than a carbon fueled SOFC system with separate carbon gasification unit and SOFC unit. They achieved a power density of 220 mW cm^{-2} at 0.68 V at 1178 K.

Since CO is participated in the electrochemical reaction, enhancing the Boudouard reaction between the CO_2 and carbon is effective in improving the performance of DC-SOFCs. The Boudouard reaction rate could be increased by increasing the operating temperature or using suitable catalyst to facilitate the reaction. However, increasing the temperature could decrease the lifetime of the DC-SOFC thus it is critical to develop suitable catalyst for Boudouard reaction at reduced temperature. Wu et al. [11] adopted Fe_mO_n-M_xO (M = Li, K, Ca) as catalyst to enhance the Boudouard reaction in SOFC anode and the peak power density was 297 mW cm^{-2} at 1123 K. Li et al. [12] and Tang et al. [13] also found that by introducing appropriate catalyst (such as Fe-based) into DC-SOFC, the operating temperature could be decreased and the performance could be improved. Bai et al. [14] studied a 3-cell DC-SOFC stack and obtained a power density of 465 mW cm^{-2} at 1123 K. They also found that the life time of the DC-SOFC and the carbon fuel utilization were both decreased with increasing current.

In addition to power generation, new DC-SOFC systems have been proposed and demonstrated to be feasible for simultaneous power and gas cogeneration. Alexander et al. [15,16] developed a steam-carbon fuel cell for simultaneous generation of H_2 and power and the efficiency was over 78%. Xie et al. [1,17] verified the CO_2 shuttling mechanism of DC-SOFCs by comparing the electrochemical characteristics of a CO-fueled SOFC with a DC-SOFC. They also proposed CO gas and electrical power co-generation by a DC-SOFC, which significantly increased the overall efficiency of the DC-SOFC.

A few groups also studied the practical applications of DC-SOFCs. Zhou et al. [18] fabricated a cathode supported tubular DC-SOFC with a continuous fuel supply to the anode. They proposed that the DC-SOFC performance could depend on the distance between the porous anode layer and the carbon bed, which was verified by our previous isothermal modeling work [19]. Jiao et al. [20] used structurally modified coal char as fuel in a DC-SOFC and found that the Boudouard reaction activity was greatly improved, which consequently improved the power output of the cell. In addition to CO_2, H_2O can also be used as a gasifying agent to convert solid carbon into gaseous CO. Lee et al. [10] compared the thermodynamic performance of DC-SOFC with H_2O gasification and CO_2 gasification and no significant difference in terms of electrical output was found. However, Ong and Ghoniem [21] developed a 1D MEA model and found that significant performance improvement could be achieved through recycling H_2O rather than CO_2 between anode and the gasifier in an indirect DCFC.

The above-mentioned studies demonstrated great potential of DC-SOFC and attempted to understand the fundamental mechanisms in DC-SOFC. However, it can also be seen that the under-

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