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Modeling of all porous solid oxide fuel cells

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HIGHLIGHTS

- A model for an all-porous solid oxide fuel cell is developed for the first time.
- Good carbon resistance of the all porous fuel cell can be achieved.
- High performance of the all porous fuel cell can be achieved with CH₄ fuel.
- Co-generation of electricity and syngas in all porous fuel cell is proposed.

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ABSTRACT

The all porous solid oxide fuel cell concept is proposed to solve the carbon deposition problem of solid oxide fuel cells. The transport of oxygen molecules from the cathode to the fuel side through the porous electrolyte can resist carbon deposition but could reduce the fuel cell performance. In this paper, a two-dimensional model for all porous solid oxide button cells is developed for the first time. After model validation with experimental data, the model is then extended for a tubular cell for parametric simulations. The effects of operating conditions and the electrolyte microstructure properties on carbon resistance and electrochemical performance of all porous solid oxide fuel cells are examined. The good carbon resistance of all porous solid oxide fuel cell is numerically demonstrated. It is found that the electrochemical performance and anode surface O/C ratio is significantly affected by anode inlet gas composition and flowrate. In addition, the anode supported all porous solid oxide fuel cell solid oxide fuel cells or bow generation and coking resistance. The results of this study form a solid foundation to understand the mechanism and promising future of all porous solid oxide fuel cells.

1. Introduction

A solid oxide fuel cell (SOFC) is one of the most attractive technology for converting the chemical energy fuels to electricity through electrochemical reactions [1–4]. Compared with other electric generators, SOFCs work in a clean, quiet and high efficiency manner. Compared with low temperature fuel cells such as proton exchange membrane fuel cells (PEMFCs) requiring very pure hydrogen fuel, SOFCs are fuel flexible and can use CO containing feeds for power generation. The utilization of carbon contained fuel in SOFCs has received more and more interest recently, including the direct utilization of solid carbon [5,6]. Methane is an interesting alternative fuel choice for SOFCs as it is a main component in biogas and natural gas. Compared with H_2 , methane has a higher volumetric energy density with lower price. Using methane as fuel can hopefully accelerate the commercialization of SOFCs for a variety of applications [7–11]. However, the direct fueling of methane causes severe coking and carbon deposition on SOFC anode (typically with nickel catalyst), resulting in catalyst deactivation [12]. Apart from designing novel anode materials [13,14], strategies like adding external reformers and introducing steam together with methane have been proposed to enable nickel based anodes for the use of methane while resisting carbon deposition [15–17]. Nevertheless, these strategies require extra auxiliary facilities and raise the total expense.

Recently, Guo et al. [18] proposed a novel concept of all porous solid oxide fuel cell (AP-SOFC). By using a porous electrolyte, part of O_2 from the cathode side can be transported to the fuel side to inhibit carbon deposition from methane fuel. In their preliminary experimental

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Nomenclature		n	number of electrons transferred per electrochemical re-
Abbreviation		N:	flux of mass transport kg m ^{-3} s ^{-1}
		n	(partial) Pressure. Pa
AP-SOFC all porous solid oxide fuel cell		$P P_{CO}^{L}$	local CO partial pressures. Pa
BSCF	barium strontium cobalt ferrite ($Ba_0 \ Sr_0 \ Co_0 \ Fe_0 \ O_{3-\delta}$)	$P_{CO_2}^L$	local CO ₂ partial pressures, Pa
CGO	gadolinium-doped ceria $(Gd_{0.1}Ce_{0.0}O_{1.0})$	$P_{\mu_{0}}^{L}$	local H ₂ partial pressures. Pa
СМО	carbon monoxide oxidization	$P_{H_{L}O}^{I_2}$	local H_2O partial pressures. Pa
HO	hydrogen oxidization	$P_{\Omega_1}^L$	local O_2 partial pressures. Pa
MO	methane oxidization	R^{O_2}	gas constant. 8.314 J·mol ^{-1} ·K ^{-1}
MSR	methane steam reforming	R_{CMO}	carbon monoxide oxidization reaction
0/C	oxygen to carbon	R _{HO}	hydrogen oxidization reaction
SCCM	standard cubic centime per minute	R _{MSR}	methane steam reforming reaction
SOFC	solid oxide fuel cell	R_{MO}	methane oxidization reaction
TPB	triple phase boundary	R _{WGS}	water gas shift reaction
WGS	water gas shift	Т	temperature, K
		u	velocity field, m ³ ·s ⁻¹
Roman		V	volume fraction
		y_i	mole fraction of component i
B_0	permeability coefficient, m ²	z	gas diffusion direction
c_{CO_2}	mole concentration of carbon dioxide, $mol m^{-3}$		
c_{H_2O}	mole concentration of water, $mol m^{-3}$	Greek letters	
$D_i^{e\!f\!f}$	effective diffusivity of species i , m ² ·s ⁻¹		
$D_{ik}^{e\!f\!f}$	knudsen diffusion coefficient of <i>i</i> , $m^2 s^{-1}$	α	charge transfer coefficient
$D_{im}^{e\!f\!f}$	molecular diffusion coefficient of <i>i</i> , $m^2 s^{-1}$	ε	porosity
E_{act}	activation energy, $J \text{-mol}^{-1}$	η_{act}	activation overpotential loss, V
E_{CO}	equilibrium potential for carbon monoxide oxidization, V	η_{ohmic}	ohmic overpotential loss, V
E_{CO}^0	standard equilibrium potential for carbon monoxide oxi-	κ	permeability, m ²
	dization, V	μ	dynamic viscosity of fluid, Pa·s
E_{eq}	equilibrium Nernst potential, V	ρ	fluid density, kg·m ⁻³
E_{H_2}	equilibrium potential for hydrogen oxidization, V	σ	conductivity, S/m
$E_{H_{2}}^{0}$	standard equilibrium potential for hydrogen oxidization, V	γ	pre-exponential factor, A m^{-2}
F	Faraday constant, 96,485 $C mol^{-1}$	τ	tortuosity
i	operating current density, $A m^{-2}$		
i _o	exchange current density, $A \cdot m^{-2}$		



Fig. 1. Schematic of a tubular all porous solid oxide fuel cell (AP-SOFC).

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