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A comprehensive CFD model of anode-supported solid oxide fuel cells

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ABSTRACT

The two-dimensional comprehensive CFD model of anode-supported SOFCs operating at intermediate temperature has been presented. This model provides transport phenomena of gas species with electrochemical characteristics and micro-structural properties, and predicts SOFC performance. The mathematical model solves conservation of electrons and ions, continuity equation, conservation of momentum, conservation of mass, and conservation of energy. A continuum micro-scale model based on statistical properties together with a mole-based conservation model was employed. CFD technique was used to solve the set of governing equations. The cell performance was decomposed with contributions of each overpotential and was presented at several operating temperatures with analysis of effective diffusivity. It was found that the contribution of potential gain due to temperature rising was considerably high. However it became non-significant at high operating temperature due to decreasing of effective diffusivity in AFL. These results showed that the performance and the distributions of current density, overpotentials, and mole fractions of gas species have a strong dependence upon temperature. From these results, it was concluded that the conservation of energy should be accommodated in comprehensive SOFC model. Also the useful information for the effect of parameters on cell performance and transport phenomena was provided.

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1. Introduction

The development of intermediate temperature solid oxide fuel cells (IT-SOFCs), operable at less than 800 °C, is presently focusing on anode-supported SOFCs by employing a thin electrolyte. Anode-supported SOFCs have been widely studied for their relatively low operating temperature, high current density and cost-effective fabrication techniques [1]. The relatively low operating temperature is attracting much interest because this feature could enhance the long-term stability of SOFC with reduced thermal degradation of electrodes due to operational sintering and could enable to use higher conductivity metal interconnects. Anode-supported SOFCs also have an advantage of high Nernst potential and low degradation of corrosion. In the development of anode-supported SOFCs, the planar-type design has received much attention because it has achieved high power density [2,3] but it has larger thermal–mechanical stresses and is more difficult to seal than the tubular-type design. The tubular-type design can be less troublesome with sealing and thermal–mechanical stresses [4] and has relatively mature design characteristics [5], but it has high manufacturing costs. The integrated-planar SOFCs (IP-SOFCs), combining the advantages of the planar and tubular design, are currently under study [6].

A theoretical investigation of SOFC has been extensively performed for the comprehensive understanding of internal phenomena and to reduce the time and effort required for experimental procedures. In this respect, numerical calculations are a very useful tool in SOFC research. Several models have been developed to simulate anode-supported SOFCs. Bessler et al. [7], Morel et al. [8], Shi et al. [9], Hussain et al. [10], Nam and Jeon [11], and Jeon et al. [12] developed a comprehensive model to provide detailed description of the electrochemical processes and transport phenomena. Yakabe et al. [2], Recknagle et al. [13], Yuan et al. [14], Bedogni et al. [15], Andreassi et al. [16], Zhu and Kee [4], and Bove and Ubertini [17] studied a species transports considering fluid behavior and electrochemical kinetics by computational fluid dynamic (CFD)-based model. Xue et al. [5], Aguiar et al. [18,19] and Iora et al. [20] predicted steady-state performance or transient behavior. Such models can be a useful tool for cell design and optimization.

In this study, the continuum micro-scale model [11,12] was extended to the flow channels considering conservation of energy to build a bridge connecting the micro-scale model to the macro-scale model. This paper provides the detailed information of two-dimensional heat and mass transport phenomena with electrochemical characteristics for intermediate temperature anode-supported SOFCs. In this model, the micro-scale model was introduced to the analysis of electrochemical process and gas

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species transport on the PEN, and CFD techniques were implemented by mole-based conservation equations.

2. Model description

The two-dimensional anode-supported SOFCs model was used to analyze the electrochemical reaction and transport phenomena which are strongly coupled with conservation of electrons and ions, continuity equation, conservation of momentum, conservation of mass, and conservation of energy. A continuum micro-scale model based on statistical properties and mole-based conservation model are employed. CFD technique is used to solve the set of governing equations. The model was assumed steady state, and isotropic/homogeneous electrode and electrolyte. Since this study was performed in two-dimensional model, the effects of interconnect rib which can be presented in three-dimensional model, i.e., contact resistance, in-plane ohmic loss, and non-uniform current generation, were not considered.

2.1. Geometry and operation

Anode-supported SOFCs are composed of PEN, interconnector and gas channel. The PEN is composed of comparatively thick anode substrate layer (ASL), anode functional layer (AFL), thin electrolyte, cathode functional layer (CFL) and cathode current collect layer (CCCL). Fig. 1(a) is a schematic representation of planar-type anode-supported SOFCs. The laminated PEN is sandwiched between interconnectors and the reactant gases are flowing through the interconnectors. This cell geometry enables two-dimensional description of the problem as shown in Fig. 1(b). The model considers seven sub-domains; anode channel (ACH), ASL, AFL, electrolyte, CFL, CCCL, cathode channel (CCH). Additional resistances due to the presence of interconnector are not considered. Wall boundaries are assumed to having a constant temperature. The fuel and air, introduced by plug flow and have co-flow configuration, come in from the inlets on the left and are transported into the pores of the electrode by dusty-gas model. The micro-scale description in PEN is illustrated in Fig. 1(c). The anode is composed of a mixture of Ni and YSZ particles and the CFL is made of mixture of LSM and YSZ. The three phase boundaries (TPBs), where the electronic and ionic particles are randomly packed with each other, are the active reaction sites and the concomitant reaction zone extends on the Ni catalyst surface due to surface diffusion (spillover) of oxide ions [21]. It is assumed that electrochemical reactions occur only on

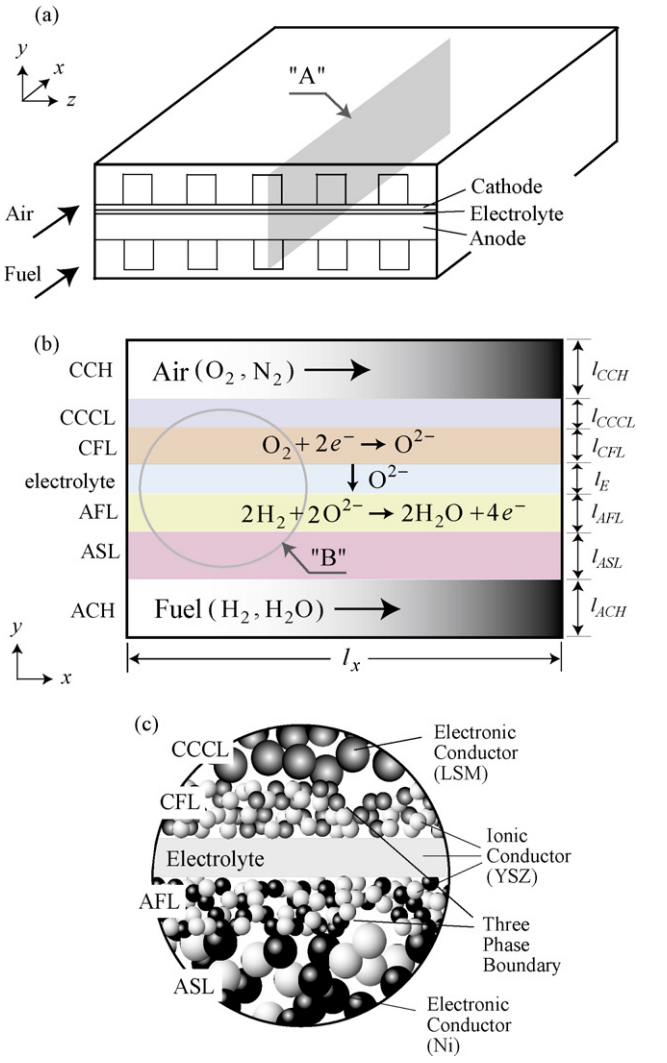

Fig. 1. (a) Schematic illustration of the unit cell of planar-type anode-supported SOFCs, (b) cross-section of anode-supported SOFCs which represents computational domain in this model (detailed "A") and (c) micro-scale description in PEN (detailed "B").

Table 1
Geometry and operating conditions.

Properties and conditions	Value or expression	
V^{cell}, T, p_t	0.7 V, 700 °C, 1 atm	
$x^0_{H_2}$, $x^0_{O_2}$	0.7, 0.21	
l_{ACH}, l_{ASL}, l_{AFL}, l_E, l_{CFL}, l_{CCCL}, l_{CCH}, l_x	1 mm, 1 mm, 20 μm, 10 μm, 15 μm, 85 μm, 1 mm, 5 cm	
ε_{ASL}, ε_{AFL}, ε_{CFL}, ε_{CCCL}	0.5, 0.25, 0.25, 0.5	
τ	3	
ϕ^A_{el}, ϕ^C_{el}	0.5	
d^{ASL}_p, d^{AFL}_p, d^{CFL}_p, d^{CCCL}_p	1 μm, 0.5 μm, 0.5 μm, 4 μm	
$\mu_{fuel(air)}$	$x_{H_2(O_2)}\mu_{H_2(O_2)} + x_{H_2O(N_2)}\mu_{H_2O(N_2)}$	(1)
$C^{fuel(air)}_p$	$x_{H_2(O_2)}C^{H_2(O_2)}_p + x_{H_2O(N_2)}C^{H_2O(N_2)}_p$	(2)
$\kappa_{fuel(air)}$	$x_{H_2(O_2)}\kappa_{H_2(O_2)} + x_{H_2O(N_2)}\kappa_{H_2O(N_2)}$	(3)
h_{form}	$\dfrac{-252.1951 + 0.067393T - 1.262354\times10^{-4}T^2 + 2.291166\times10^{-8}T^3}{1 - 1.250512\times10^{-4}T + 4.599617\times10^{-7}T^2}$	(4)
u_{fuel}, u_{air}	5 ms^{-1}, 13 ms^{-1}	
θ_c	30°	
κ_A, κ_E, κ_C	6 W m^{-1} K, 2.7 W m^{-1} K, 11 W m^{-1} K	

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