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3-D model of thermo-fluid and electrochemical for planar SOFC

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Abstract

A numerical simulation tool for calculating the planar solid oxide fuel cells was described. The finite volume method was employed for the simulation, which was on the basis of the fundamental conservation laws of mass, momentum, energy and electrical charge. Temperature distributions, molar concentrations of gaseous species, current density and over potential were calculated using a single cell unit model with double channels of co-flow and counter-flow cases. The influences of operating conditions and anode structure on the performances of SOFC were also discussed. Simulation results show that the co-flow case has more uniform temperature and current density distributions and smaller temperature gradients, thus offers thermostructural advantages than the counter-flow case. Moreover, in co-flow case, with the increasing of delivery rate, temperature and hydrogen mass fraction of fuel, average temperature of PEN, current density and activation potential also rise. However, with increasing the delivery rate of air, average temperature of PEN decreases. In particular, it is effective to improve the output voltage by reducing the thickness of anode or increasing its porosity.

Keywords: Planar SOFC; Thermo-fluid model; Electrochemical model; Temperature field; Current density; Over potential

1. Introduction

The solid oxide fuel cell (SOFC) has been drawn attention because of its higher energy conversion efficiency, power density, low environmental hazards and production cost. Thus, the SOFC is expected to reach commercialization in a few years and could be a promising alternative energy source for residential and distributed power plants in the 21st century [1–3]. However, further development of the planar SOFC faces challenges related to maximizing the power density and minimizing the non-uniform distribution of temperature, which contributes to thermal stress in the SOFC components [4–5].

The temperature and current density distributions in a SOFC are determined by the working conditions, such as the delivery rates and temperatures of the fuel and air to the system. Fuel utilization and fuel distribution are also critical due to the exothermic electrochemical reactions. Increased fuel flow tends to increase the uniformity of the reaction rates across the active area and decrease fuel utilization. Decreased fuel flow tends to increase the fuel utilization, but can cause local fuel depletion and cold spots that exacerbate temperature non-uniformities. Air and fuel inlet temperatures also affect the reaction rates, cell temperature and fuel utilization. Therefore, management of the flow of air and fuel and the distribution of each, is critical to the stable operation of the cell [5]. Other factors that affect the temperature distribution and fuel utilization are the thickness and porosity of the anode. As a consequence, the geometrical design of SOFC is important in establishing a well-operating cell. In order to efficiently develop planar SOFC stacks, it is convenient and effective to have the capability to experiment numerically with the effects of different geometric designs on the operation and performance.

In the past, modeling of the planar SOFC during steady operation to calculate the temperature and current density distributions has been reported [6–12]. Investigations of planar SOFC operation and planar SOFC performance have predicted cell temperature and current distribution for various flow patterns [13–14]. However, only less work has been performed on the influences of variation of structure and operating conditions on the performance of SOFCs [15]. The purpose of present work is to demonstrate a model to predict temperature distributions, species concentrations, current density and

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Nomenclature

C_k	concentration of component k
C_p	specific heat (J kg^{-1} K^{-1})
$D_{k,eff}$	effect diffusivity of component k (m^2 s^{-1})
E_f	internal energy of mixture gas (J)
E_s	internal energy of solid (J)
F	Faraday constant (C mol^{-1})
I	local current density (A/cm^2)
I_k	mass source of mixture component k
j	transfer current density (A cm^2)
k_{eff}	effect thermal conductivity coefficient (W m^{-1})
k_f	thermal conductivity coefficient of gas (W m^{-1})
k_s	thermal conductivity coefficient of solid (Wm^{-1})
K	permeability coefficient (m^2)
P	pressure of mixture (Pa)
R	gas constant (J mol^{-1} K^{-1})
s_k	reaction coefficient of component k
S_E	energy source (J)
S_M	momentum source
ΔS	entropy change (J mol^{-1})
T	Temperature (K)
U	mixture velocity (m/s)

Greek letters

δ	anode thickness (m)
ε	porosity
$\eta_{act,a}$	activation potential at anode (V)
$\eta_{act,c}$	activation potential at cathode (V)
η_{conc}	concentration potential (V)
μ_{eff}	effect viscosity
ρ	density (kg m^{-3})
σ_{eff}	effect electrical conductivity (Ω^{-1} m^{-1})

over potentials. In this study, co- and cross-flow cases were examined. In particular, the effects of the structural parameters and the operating conditions on the performance of a SOFC are discussed in a co-flow case, such as thickness and porosity of anode, delivery rates and temperatures of fuel and air.

2. Mathematics model

2.1. Model geometry

Generally, the repeating unit of a typical planar SOFC stack is constructed of a positive electrode–electrolyte–negative electrode (PEN) and an interconnector plate "stacked" together. For the sake of simplicity of calculation, one repeating cell unit, which includes a PEN, air and fuel channels and 1/2 interconnect thickness top and bottom in the *Y*-direction, was analyzed in this simulation. The one-cell stack and the single unit model are illustrated in Fig. 1. In this model, the thicknesses of anode, cathode, electrolyte and interconnect were 0.5, 0.25, 0.05 and 1.0 mm, respectively.

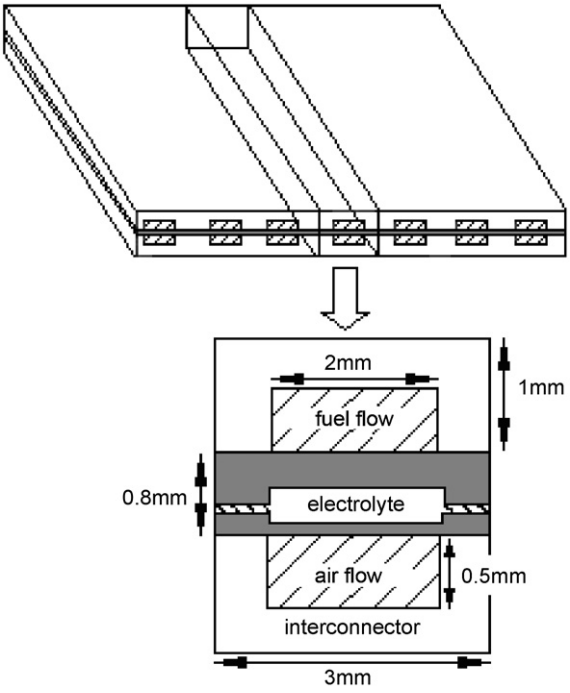

Fig. 1. Illustrations of the one cell-stack and singe cell unit model.

2.2. Thermo-fluid model

The ANSYS-CFX code was selected to solve the thermo-fluid model. In the simulation, the solid and fluid domains were divided into some discrete meshes, and in each computational mesh, the conservation equations of species, mass, momentum and energy were solved using the finite volume method.

In general, gas species transfer mainly by convection in the flow channels and diffusion in the porous electrodes. The species conservation equation:

$$\nabla(\rho C_k U) = \nabla(D_{k,eff}\nabla C_k) + I_k, \quad k = H_2, O_2, H_2O \tag{1}$$

where I_k is the rate of production or consumption of specie k, and given by [16]:

$$I_k = \pm\frac{s_k j}{2F} \tag{2}$$

The diffusion coefficients of hydrogen and oxygen are obtained as follow [16]:

$$D_{O_2} = 0.181 \times \left(\frac{T}{273}\right)^{1.5}, \qquad D_{H_2} = 0.753 \times \left(\frac{T}{273}\right)^{1.5} \tag{3}$$

The mass conservation equation:

$$\nabla \cdot (\varepsilon\rho U) = 0 \tag{4}$$

Both the air and fuel flows were considered as ideal gas mixtures with the density given by:

$$\rho = \frac{P}{RT}\left(\sum_k \frac{m_k}{M_k}\right) \tag{5}$$