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Design and numerical analysis of a planar anode-supported SOFC stack

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ABSTRACT

In the present study, numerical simulations are conducted to examine the flow characteristics and attributes of electrochemical reactions in the stack through three-dimensional analysis using finite volume approach prior to the fabrication of the SOFC stack. The stack flow uniformity index is employed to investigate the flow uniformity whereas in the case of electrochemical modeling, different mathematical models are adopted to predict the characteristics of activation and ohmic overpotentials that occur during electrochemical reactions in the cell. The normalized mass flow rate is found almost same in each cell with flow uniformity index of 0.999. The calculated voltage and power curves under different average current densities are compared with experimental results for the model validation. The changes in the voltage and power of the SOFC stack, current density, temperature, over potential and reactants distributions in relation to varying amounts of reactants flow are also examined. The current density distribution in each cell is observed to vary along the anode flow direction. The temperature difference in each cell is almost same along the flow direction of reactants, and the irreversible resistance showed an opposite trend with a temperature distribution in each cell.

1. Introduction

A fuel cell is an energy transformation device that directly converts the chemical energy produced by fuel into electrical energy through an electrochemical reaction. This device is highly efficient, presents little noise because it has no driving device, lends itself to easy assembly and varying capacities by modulation, and causes no pollution. These properties have directed considerable attention to fuel cells as a next-generation energy source. Unlike a battery, a fuel cell is supplied with fuel from an external supply device and continuously generates electricity [1,2].

Fuel cells are differentiated according to the fuel, oxidant, electrolyte, operating temperature, and electrode used. The solid oxide fuel (SOFC) is one of the promising types of the fuel cell which generally operates at high temperatures ranging from 700 to 1000 °C. Therefore, it is characterized by generation efficiency higher than that observed in other fuel cells. The representative types of SOFC include planar, cylindrical and flat-tubular. The advantage of a planar SOFC is its low electrical resistance because of the short movement path traversed by electrons, easy assembly of stack modules that are immediately available for long-term driving, and high efficiency. Its disadvantage is that it presents difficult sealing given differences in the thermal expansion coefficients of ceramic cells and metal materials at high temperature during stacking [3,4].

There are several articles about computational analysis for SOFC stack because it is important to predict the performance of SOFC stack before the fabrication. E. Achenbach [5] and P. Costamagna et al. [6] proposed experimental formulas for activation overpotential and performed three-dimensional analyzes of temperature distribution and performance changes in a unit cell and stack. K. P. Recknagle et al. [7] carried out a three-dimensional heat and flow analysis of a planar SOFC. These authors considered electrochemical reaction and predicted the temperature and the current density distribution of the planar SOFC. They also predicted the concentration distribution of reactants (H_2 and O_2) on the basis of the diverse flow forms (co-flow, counter-flow, and cross-flow configurations) within the electrodes. J. R. Ferguson et al. [8] analytically examined the effects of the heat and mass transfer on

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Nomenclature

Roman symbols

C_i	Inertial resistance factor of species [m^{-1}]
C_p	Isobaric heat capacity [$J\ mol^{-1}\ K^{-1}$]
d_p	Particle size [m]
d_{pore}	Pore size [m]
D_{eff}	Effective diffusion coefficient [$m^2\ s^{-1}$]
D_{ij}	Binary diffusion coefficient of species [$m^2\ s^{-1}$]
$D_{K,i}$	Knudsen diffusion coefficient of species [$m^2\ s^{-1}$]
E	Energy [J]
E^0	Standard state potential [V]
E^{act}	Activation energy [$kJ\ mol^{-1}$]
E_{rev}	Reversible potential [V]
F	Faraday constant [96485.3 $C\ mol^{-1}$]
h_i	Enthalpy of species [$J\ kg^{-1}$]
I	Current density [$A\ m^{-2}$]
I^0	Exchange current density [$A\ m^{-2}$]
$\overrightarrow{I}$	Unit vector
I_{cell}	Total current through the cell [A]
I_{avg}	Average current density [$A\ m^{-2}$]
$\overrightarrow{J}_i$	Diffusion flux of species [$kg\ m^{-2}\ s$]
k_i	Heat conductivity of species [$W\ m^{-1}\ K^{-1}$]
k_{eff}	Effective heat conductivity [$W\ m^{-1}\ K^{-1}$]
K_i	Permeability [m^2]
m'	Normalized mass flow rate
$\dot{m}$	Mass flow rate [$kg\ s^{-1}$]
Mw_i	Molecular weight of species [$kg\ mol^{-1}$]
p	Pressure [Pa]
P_i	Partial pressure of species [bar]
R	Universal gas constant [8.314 $J\ mol^{-1}\ K$]
R^{act}	Activation impedance [$\Omega\ m^2$]
R_{irr}	Irreversible resistance [$\Omega\ m^2$]
R^{ohm}	Ohmic resistance [$\Omega\ m^2$]
s_i	Entropy of species [$J\ K^{-1}$]
T	Temperature [K]
U	Stack flow uniformity index
$\overrightarrow{v}$	Velocity vector
V_{cell}	Cell voltage [V]
V_{mol}	Molecular volume [m^3]
X_i	Mole fraction of species
Y_i	Mass fraction of species

Greek symbols

α	Transfer coefficient
δ	Thickness [m]
ε	Porosity
γ_{an}	Pre-exponential factor of anode [$A\ m^{-2}$]
γ_{ca}	Pre-exponential factor of cathode [$A\ m^{-2}$]
η^{act}	Activation over potential [V]
η^{ohm}	Ohmic over potential [V]
μ	Dynamic viscosity [Pa s]
ρ	Density [$kg\ m^{-3}$]
σ	Electrical or ionic conductivity [$S\ m^{-1}$]
τ	Tortuosity
$\overline{\overline{\tau}}$	Stress tensor

fuel cell performance in a planar SOFC. They proposed temperature dependent experimental expressions for electrical conductivities of the anode electrode, a cathode electrode, electrolyte, and interconnect of the planar SOFC. F. Arpino et al. introduced a robust mathematical model and finite element-based numerical approach to calculate the heat and mass transfer phenomenon in the SOFC [9]. N. F. Bessette et al. [10] conducted a numerical analysis of an SOFC stack module and compared the output characteristics of the unit cell and the stack. They revealed that the unit cell constituting the stack have output characteristics that differ from those of the stack, and by using the calculation result for a unit cell to predict the output characteristics of an SOFC stack module is an inaccurate approach.

In the present analysis, a numerical analysis of a 5-cell planar Solid Oxide Fuel Cell (SOFC) stack is conducted in order to confirm the flow uniformity of supplied reactants in the stack, and to calculate the electrochemical reactions. To effectively conduct a three-dimensional computational analysis of the SOFC stack, ANSYS Fluent is used and an in-house code (User Defined Function) is employed to calculate electrochemical reactions. In order to confirm the flow uniformity for the present SOFC stack, the stack flow uniformity criteria is applied. In order to validate the modeling, I–V–P curves of simulated results are compared with experimental data. The temperature and the current density distributions in the cells are also examined by varying reactant flow rates. The voltage drop in the cells is also observed on the basis of reactants concentration and irreversible resistances.

2. Geometry and calculation conditions

2.1. Geometry and mesh generation

The overall shape of the SOFC stack is shown in Fig. 1. The KIER and MAGNEX CO. designed and fabricated a planar SOFC stack, which comprises of five planar cells, separators, spacers, mica, and other components, and its internal flow is of cross-flow type. The cells are arranged in concentric circles as a core part in order to directly produce electricity through supplied reactants. Five cells are stratified in the stack, in which as many separators as cells are installed. The shape of the separator is displayed in Fig. 2. These separators serve as the flow paths traversed by the reactants and products, also, they induce electricity flow. It is assumed that the shape of the flow paths is indicative of the separators being porous media in order to save the simulation time. The planar SOFC stack used in this study is sealed using mica which possesses excellent electrical insulation and gas-sealing capabilities that enable to maintain the sealing efficiency of the stack under high temperature and humidity. The stack module is assembled using metal spacers to strengthen tolerance between the cells during stacking. Such design technology (i.e., features the use of non-glass seals) for SOFC stacks enables easy maintenance and repair, as well as ready linkage with a system because of the stack's compact composition.

Fig. 3 shows a grid for numerical simulation of the SOFC stack. The grids are generated by considering only the internal flow region of the overall shape in Fig. 1, and the grids are converted into dense units centered on an anode electrode, cathode electrode,