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A three-dimensional model for transient performance of a solid oxide fuel cell

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ABSTRACT

This paper presents an analysis of transient behavior of an anode-supported solid oxide fuel cell (SOFC) using a model, which has recently been built for steady state operation. The model is three dimensional (3D), which takes into account heat and mass transport, chemical and electrochemical reactions taking place simultaneously in the cell. The electrochemical processes are assumed to take place in a layer of finite thickness at electrode–electrolyte interfaces. A repeating unit of a planar anode-supported SOFC with co-flow configuration is investigated. Step changes of working voltage and fuel composition are applied to the cell. Results for the dynamic profiles of the temperature, the current density and the activation overpotential distributions in the cell are presented and discussed.

Introduction

Solid oxide fuel cells (SOFCs) generate electricity directly from a gaseous fuel at high temperatures (500–1000 °C) in an environmentally-friendly way. They possess a number of advantages even compared with other fuel cell types such as fuel flexibility, no need for expensive catalysts, geometrical flexibility, and the capability of working in a co-generation energy system [1].

When working in a co-generation energy system, SOFCs would yield higher efficiency, however, they could frequently be subjected to unstable working conditions such as changes in load demand and potential uncertainties/failures happening to any components of the system. Therefore, a thorough understanding of dynamic behaviors of SOFCs is indispensably important. Indeed, a number of studies on SOFC dynamics has been done and published in the open literature using numerical approaches [2–15]. Among those, many have used system/lumped models with an objective of dynamic control of SOFCs working in a power generation system [2–6]. Qi et al. [7,8] employed a cell-level species dynamic model, in which a finite volume of constant temperature and pressure representing a whole tubular cell was analyzed. One-dimensional (1D) models have also been employed by different researchers [9–11]. Damme and Fedorov [9] investigated the transient characteristics of a planar SOFC such as the total time required for startup of the cell from ambient temperatures and the maximum temperature gradients developed during the process. Gemmen and

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Nomenclature

A_{ac}	active area per unit volume, m^{-1}
$\bar{c}$	constant-volume specific heat, J kg^{-1}
C	charge concentration, C m^{-3}
$C^{\star}$	effective concentration, C m^{-3}
d	particle diameter, m
D	diffusion coefficient, m^2 s^{-1}
e	specific internal energy, J kg^{-1} K^{-1}
E	potential, V
F	Faraday constant, 96,487 C mol^{-1}
$F_{m,j}$	diffusive mass flux of species m, kg m^{-2} s^{-1}
$F_{h,j}$	diffusive energy flux component, J m^{-2} s^{-1}
i	current density, C m^{-2} s^{-1}
i_0	exchange current density, C m^{-2} s^{-1}
j	transfer current per unit volume, C m^{-3} s^{-1}
k	thermal conductivity, W m^{-1} K^{-1}
$k_{0,a}$, $k_{0,c}$	reaction rate coefficient, mole m^{-3} s^{-1} V^{-1}
K_i	permeability of porous media, kg m^{-3} s^{-1}
p	pressure, Pa
r	reaction rate, mole m^{-3} s^{-1}
R	universal constant of gas, 8.314 J mol^{-1} K^{-1}
R_e	electrochemical reaction rate, mole m^{-3} s^{-1}
Q_c	chemical heat source, J m^{-3} s^{-1}
Q_e	electrochemical heat source, J m^{-3} s^{-1}
Q_ohm	Joule heating, J m^{-3} s^{-1}
s_i	momentum source component, kg m^{-2} s^{-2}
s_m	production/consumption rate of species m, kg m^{-3} s^{-1}
s_Σ	total mass source, kg m^{-3} s^{-1}
T	temperature, K
u_i	velocity component, m s^{-1}
U_i	superficial velocity component, m s^{-1}
x_i	Cartesian coordinate, m
Y_m	mass fraction of component m

Greek letters

β	symmetry factor, 0.5
ε	porosity
η	overpotential, V
μ	dynamic viscosity of gas, kg m^{-1} s^{-1}
Φ	potential, V
ρ	gas mixture density, kg m^{-3}
τ	tortuosity
τ_{ij}	stress tensor, Pa
σ	ionic/electric conductivity, Ω^{-1} m^{-1}

Subscripts

m, n	species index
i, j, k	cartesian directions

Abbreviations

ADL	anode diffusion layer
ACL	anode catalyst layer
CDL	cathode diffusion layer
CCL	cathode catalyst layer

Johnson [11] analyzed the dynamic characteristics of SOFCs of both planar and tubular designs and found that a reverse current could happen over a significant portion of the cell over a period of time. They then suggested further examination of current reversal because of potential risk for electrode degradation. In these models, transversal variations were neglected and/or groups of cell components (channel/interconnect, electrodes/electrolyte) were assumed to possess the same temperature. However, the transversal variations have been taken into account in two-dimensional (2D) models [12–15]. Xie and Xue [12] used an isothermal model for a button type anode-supported SOFC. Serincan et al. [14] utilized the commercial multiphysics software COMSOL to analyze the transient behaviors of a micro-tubular SOFC. Tseronis et al. [15] introduced a model for predicting SOFC performance at both steady and dynamic states.

Additionally, a couple of three-dimensional (3D) models have recently been developed for transient performance of SOFCs [16–18]. Chaisantikulwat et al. [16] adopted a 3D model using COMSOL for a planar anode-supported SOFC with counter-flow configuration. Temporal variation of the output voltage, chemical species fluxes at the outlets and the temperature averaged over the cathode–electrolyte interface resulting from step changes in the current density and the fuel concentration was analyzed. It was found that the response time of the temperature is approximately 400 s. In the work of Peksen et al. [17], a thermomechanical analysis of a planar type SOFC short stack was conducted based on a predicted temperature profile. Focus was put on the transient thermal behavior of the stack and its thermomechanical response during the heating-up, operation and shut-down stages. Menon et al. [18] used a quasi-2D/3D combined model to analyze the transient behavior of a stack consisting of 30 planar anode-supported cells. Various results for the current density, activation, etc. in a unit cell and temperature in the stack in response to step changes in both current and voltage were reported.

The objective of the current work is to analyze transient characteristics of an anode-supported solid oxide fuel cell using a numerical model, which has recently been built for steady state operation of SOFCs by Ho et al. [19]. The model is non-isothermal and three-dimensional using a single computational domain for the whole cell, therefore, there is no need for internal boundary conditions. The idea of using a single domain can also be found in Pasaogullari and Wang [20]. This makes it possible to solve all the transport, chemistry and electrochemistry simultaneously. Moreover, in the built model, the electrochemical reactions are assumed to take place in a catalyst layer adjacent to the electrode–electrolyte interfaces. It is physically reasonable when composite electrodes are used. This concept has been employed by several authors such as Pasaogullari and Wang [20], Nam and Jeon [21] and Zhu and Kee [22], among others, for steady state operation of SOFCs. However, there has not been so far any work using it for transient modeling of SOFCs. Additionally, with this detailed model, transient of local parameters such as temperature, current density, etc. can be observed whereas only cell-averaged ones have been presented in most of the aforementioned studies.