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Three-dimensional dynamic modeling and transport analysis of solid oxide fuel cells under electrical load change

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ABSTRACT

The aim of this study is to elucidate the transient behavior of thermodynamic variables in a solid oxide fuel cell (SOFC) upon electrical load change, which can be used for optimizing cell microstructure and developing a reliable SOFC stack design. To overcome the insufficient durability and large performance degradation, SOFC technologies still need reliable cell microstructure and stack design prior to their market deployment. This is of significant concerns when considering actual operating conditions, in particular, sudden and severe electrical load change. Enhancing the dynamic stability of SOFC is essential to improve its durability under the electrical load change. To meet the needs, the local thermodynamic state and thermo-fluid environment should be examined in detail, which requires high-fidelity numerical simulations. In this study, a physical model is developed to resolve temporally and spatially reactions and transport phenomena taking place inside planar, anode-supported SOFC stacks. The model is validated by using in-house experimental measurements of a current response profile upon electrical load change. Then, the dynamic response of thermodynamic variables upon electrical load change is investigated by assuming potentiodynamic conditions. The results of this study show that the electrical current responds excessively to the potential steps and recovers its magnitude asymptotically to the quasi-steady state. A relaxation time is needed for its dynamic response and recovery. This is explained by the time-dependent variation of the electrochemical reaction zone and species transport in the anode. The former reacts quickly to electrical load change, influencing the hydrogen concentration, while the latter shows time-delay, affecting the diffusion of hydrogen between the reaction zone and fuel channel. The time-delay required for the response of hydrogen diffusion corresponds to the relaxation time needed for the electrical current response. These results indicate that the overall transient behavior is predominantly governed by species diffusion in the anode. The pressure field also shows similar trend of time-dependent variations, whereas the temperature does not change as much as other variables, implying that it needs much longer time to adjust itself to a new operating condition.

1. Introduction

Nowadays, alternative energy technologies such as fuel cells have gained great interest given the needs for an environmentally-benign energy platform. Extensive research and development studies have been conducted to demonstrate their feasibility in the energy market [1]. Various types of fuel cell technologies have been considered, although they are all based on selective ion transport through an electrolyte and electrochemical reactions on electrodes. Fuel cells are normally classified into several groups based on the type of reactants used (e.g., hydrogen, methanol, methane, carbon monoxide, and other organic substances, etc.); electrolyte materials (e.g., acid or alkali, liquid or solid), and an operating temperature. Depending on electrolytes and operating temperature, Alkaline Fuel Cell (AFC), Proton Exchange Membrane Fuel Cell (PEMFC), Direct Methanol Fuel Cell (DMFC), Phosphoric Acid Fuel Cell (PAFC), Molten Carbonate Fuel Cell (MCFC), and Solid Oxide Fuel Cell (SOFC) technologies have been developed in the past decades (see Supplementary Table S1). Among them, low temperature PEMFC [2–4] and high-temperature SOFC [5,6] have been shown to exhibit likelihood for market deployment, attributed to their high performance and versatile applications.

Both of them have strengths and weaknesses, leading to different core applications. PEMFC has a high power density, short start-up time, low operating temperature, and simple mechanical design for easier handling [4,7]. Such features make PEMFC suitable for portable devices and mobile units (i.e., fuel cell electric vehicles) [8–10]. However, it is

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Nomenclature

E	activation energy [J·mol^{-1}]
D_{ij}	binary diffusivity between species i and j [m^2·s^{-1}]
$\dot{Q}$	charge-carrier source [A·m^{-3}]
σ	charged-species conductivity [S·m^{-1}]
i	current density [A·m^{-2}]
$\overrightarrow{F_{Da}}$	Darcy's friction force [N·m^{-3}]
ρ	density [kg·m^{-3}]
Σ_i	diffusion volume of species i [s$^{4.5}$·K$^{2.625}$·mol$^{0.75}$·kg$^{-2.25}$·m$^{-1.5}$]
D_i	diffusivity of species i [m^2·s^{-1}]
μ_i	dynamic viscosity of species i [kg·m^{-1}·s^{-1}]
ϕ	electric potential [V]
Δs^o	entropy change of reactions [J·mol^{-1}·K^{-1}]
F	Faraday constant [C·mol^{-1}]
R	gas constant [J·mol^{-1}·K^{-1}]
$\dot{H}$	heat source [W·m^{-3}]
h	height [m]
$D_{Kn,i}$	Knudsen diffusivity of species i [m^2·s^{-1}]
L	length [m]
ω_i	mass fraction of species i [–]
$\dot{R}_i$	mass production rate of species i [kg·m^{-3}·s^{-1}]
$\dot{W}$	mass source [kg·m^{-3}·s^{-1}]
$D_{mix,i}$	mixture averaged diffusivity of species i [m^2·s^{-1}]
N_i	molar concentration of species i [mol·m^{-3}]
$\dot{n}_i$	molar flux of species i [mol·m^{-2}·s^{-1}]
x_i	molar fraction of species i [–]
M_i	molecular weight of species i [kg·mol^{-1}]
η	overpotential [V]
ζ	permeability [m^2]
r_{pore}	pore size of the porous media [m]
ε	porosity [–]
A	pre-exponential factor [S·K·m^{-1}]
S	reaction site area per unit volume [m^{-1}]
$C_{p,solid}$	specific heat capacity of solid materials [J·kg^{-1}·K^{-1}]
$C_{p,i}$	specific heat capacity of species i [J·kg^{-1}·K^{-1}]
λ_{solid}	thermal conductivity of solid materials [W·m^{-1}·K^{-1}]
λ_i	thermal conductivity of species i [W·m^{-1}·K^{-1}]
l	thickness [m]
t	time [s]
τ	tortuosity [-]
$\vec{u}$	velocity [m·s^{-1}]
$\theta_{E.C.}$	volume fraction of electronic conductor in the composite [–]
w	width [m]

Acronyms

AFL	anode functional layer
ASL	anode support layer
CCCL	cathode current collecting layer
CFL	cathode functional layer
CCL	current collecting layer
EL	electrolyte
CH	gas channel
IC	interconnects
IL	interlayer

Subscripts

act	activation
a	anode
c	cathode
elec	electronic
ion	ionic
rev	reversible

Superscripts

eff	effective
0	standard

highly sensitive to impurities of hydrogen (i.e., carbon monoxide), needs expensive membrane and catalyst materials, uses complex gas diffusion and flow fields, and requires water treatment to avoid fouling and lower conductivity [1–3,11]. On the other hand, SOFC provides numerous benefits in converting fuel's chemical potential to electrical energy such as high energy conversion efficiency of 60% or higher, fuel flexibility (i.e., direct utilization of hydrocarbons as well as hydrogen), high energy density, high-quality heat supply, use of relatively inexpensive ceramic materials, nearly-zero carbon emission, and small footprints required for installation [12]. All these strengths make SOFC as an attractive choice for utility and industrial power supply and distributed power generation [13]. However, insufficient durability and large performance degradation of SOFC stacks are still remained as barriers that need to be overcome prior to their commercialization.

Especially, dynamic stability of SOFC upon varying electrical load conditions is a critical issue in determining their feasibility for market deployment. A number of factors have been taken into account to resolve such problems [14–16], which includes electrochemical (i.e., brittleness of ceramic materials upon chemical stresses), mechanical (i.e., crack propagation and fracture under severe operating conditions), and thermal (i.e., formation of hot-spot/cold-spot and fatigue failure due to thermal stresses) issues. All of these are of significant concerns when considering actual operating conditions, in particular, sudden and severe electrical load change. Such abrupt electrical load change may result in a shock-wave impact on the electrochemical, mechanical, and thermal stability of unit-cells and stacks. To address the dynamic stability issues of SOFC, it is essential to elucidate its dynamic response to electrical load change, for which coupling of electrochemical reactions and the transport of mass, momentum, and thermal energy should be temporally and spatially considered in the fuel cell model [17,18]. Note that it is extremely difficult to obtain *in-situ*, *operando* measurements for such complex phenomena because of high temperature and sealing conditions [19]. In this regard, high-fidelity numerical simulation and solver play a key role in examining the dynamic response of SOFC to electrical load change [20–22], especially high-dimensional real-time modeling approaches [23,24].

Although a significant number of modeling studies, both in static [25–35] and dynamic [36–48] analyses, have been performed, time-dependent three-dimensional simulations have not been considered as much as steady-state investigation [20]. Table 1 summarizes representative dynamic modeling studies for SOFCs selected from the literature. To reduce computational costs, lumped-transient zero-dimensional analyses were conducted. Padulles et al. developed a species dynamic model for their stack and power conditioner simulations to achieve safe and durable cell operation [36]. Zhu et al. applied the dynamic model of Padulles et al. to simplify transient simulations for a micro-turbine and fuel cell [37]. Murshed et al. neglected all the spatial resolution to comprehend dynamics of system components including a heat exchanger, reformer, and after-burner [49]. This approach was typically applied to estimate hybrid SOFC operations such as SOFC-gas turbine (GT). Zhang et al. proposed a dynamic model for a hybrid system integrated with SOFC and recuperative GT [50]. Speidel et al. studied combination of sewage sludge fermentation and gasification [51], and Zabihian et al. investigated the effect of an alternative fuel