



The effect of fuel utilization on heat and mass transfer within solid oxide fuel cells examined by three-dimensional numerical simulations



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ABSTRACT

The thermo-fluid reacting environment and local thermodynamic state in solid oxide fuel cell (SOFC) stacks were examined by using three-dimensional numerical simulations. Enhancing the performance and durability of the SOFC stacks is essential when a high fuel utilization scheme is implemented to increase the system efficiency and lower system operating costs. In this study, numerical simulations were conducted to elucidate the effect of fuel utilization on heat and mass transfer as the fuel utilization is raised. A high-fidelity three-dimensional physical model was developed incorporating elementary electrochemical reaction kinetics by assuming rate-limiting steps and spatially-resolved conservation equations. The model considers planar anode-supported SOFC stacks and is validated against their electrochemical performance experimentally measured. A parametric study with respect to fuel utilization was conducted by varying a fuel flow rate while maintaining other operating conditions constant. Results show that, when increasing the fuel utilization, a narrow and non-uniform electrochemical reaction zone is observed near the fuel inlet, resulting in substantial depletion of hydrogen in the downstream fuel flow and thus raising the partial pressure of oxygen in the anode. This subsequently lowers the electrochemical potential gradient across the electrolyte and hence induces a large gradient of ionic current density along the cell. Convective flow through porous electrodes also results in pressure gradients in the direction of both cell thickness and length. In addition, the heat balance between conduction through metallic interconnects, convection by gases and the heat generated from charged-species transport and electrochemical reactions determines a temperature gradient along the cell and its maximum location. All of these gradients may induce chemical, mechanical and thermal stresses on SOFC materials and corresponding degradation.

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1. Introduction

The recent development of solid oxide fuel cell (SOFC) stacks requires elucidating their thermo-fluid reacting environment and local thermodynamic state with an aid of high-fidelity numerical models. Given their high energy conversion efficiency of 60% or higher, fuel flexibility (i.e., direct utilization of hydrocarbon fuels) and small footprints required for installation [1], SOFCs have been proposed as a promising technology for clean power production, in particular, distributed power generation sources. To produce large-capacity electrical power, a SOFC system in general is comprised of modules stacked with large-area cells which are connected in series. In this case, defects appearing on a single cell can affect the

performance of other stacked cells and make the entire system highly deteriorated. It is important to enhance the durability of each cell in the SOFC stacks, which is significantly influenced by their thermo-fluid reacting environment and local thermodynamic state in the vicinity of the cell. Their effect is much more evident when a high fuel utilization scheme is implemented to increase the energy conversion efficiency and reduce system operating costs. High fuel utilization can result in large thermal/mechanical/chemical gradients along the cells, and hence induce corresponding stresses and affect the sealant stability [2]. Therefore, the thermo-fluid reacting environment and local thermodynamic state should be examined prior to engineering the stack design that enables reducing these gradients and stresses when the fuel utilization is raised [3,4]. However, it is substantially difficult to measure experimentally the phenomena taking place inside the SOFC stacks due to their high operating temperature (600 °C – 1000 °C)

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Nomenclature

E	activation energy [J·mol ⁻¹]	S	reaction site area per unit volume [m ⁻¹]
D_{ij}	binary diffusivity between species i and j [m ² ·s ⁻¹]	$C_{p,i}$	specific heat capacity of species i [J·kg ⁻¹ ·K ⁻¹]
Q	charge-carrier source [A·m ⁻³]	γ_0	sticking probability [-]
σ	charged-species conductivity [S·m ⁻¹]	Γ	surface site density [mol·m ⁻²]
α	charge-transfer coefficient for anode reactions [-]	λ_{solid}	thermal conductivity of solid materials [W·m ⁻¹ ·K ⁻¹]
β	charge-transfer coefficient for cathode reactions [-]	λ_i	thermal conductivity of species i [W·m ⁻¹ ·K ⁻¹]
i	current density [A·m ⁻²]	t	thickness [m]
\vec{F}_{Da}	Darcy's friction force [N·m ⁻³]	τ	tortuosity [-]
ρ	density [kg·m ⁻³]	\vec{u}	velocity [m·s ⁻¹]
Σ_i	diffusion volume of species i [s ^{4.5} ·K ^{2.625} ·mol ^{0.75} ·kg ^{-2.25} ·m ^{-1.5}]	$\theta_{E,C}$	volume fraction of electronic conductor in the composite [-]
D_i	diffusivity of species i [m ² ·s ⁻¹]	$\theta_{p,F}$	volume fraction of the pore-former in the anode support layers [-]
μ_i	dynamic viscosity of species i [kg·m ⁻¹ ·s ⁻¹]	w	width [m]
ϕ	electric potential [V]		
e^-	electron [-]		
Δs	entropy change of reactions [J·mol ⁻¹ ·K ⁻¹]		
K_i	equilibrium constant of reaction i [-]	Acronyms	
i_0	exchange current density [A·m ⁻²]	AFL	anode functional layer
F	Faraday constant [C·mol ⁻¹]	ASL	anode support layer
R	gas constant [J·mol ⁻¹ ·K ⁻¹]	CCCL	cathode current collecting layer
\dot{H}	heat source [W·m ⁻³]	CFL	cathode functional layer
h	height [m]	CCL	current collecting layer
$D_{Kn,i}$	Knudsen diffusivity of species i [m ² ·s ⁻¹]	EL	electrolyte
O_O^X	lattice oxygen [-]	CH	gas channel
L	length [m]	IC	interconnects
ω_i	mass fraction of species i [-]	IL	interlayer
\dot{R}_i	mass production rate of species i [kg·m ⁻³ ·s ⁻¹]		
\dot{W}	mass source [kg·m ⁻³ ·s ⁻¹]	Subscripts	
$D_{mix,i}$	mixture averaged diffusivity of species i [m ² ·s ⁻¹]	act	activation
x_i	molar fraction of species i [-]	a	anode
M_i	molecular weight of species i [kg·mol ⁻¹]	c	cathode
n	number of electrons generated by the overall reactions [-]	des	desorption
$V_{\dot{O}}$	oxygen vacancy [-]	elec	electronic
η	overpotential [V]	ion	ionic
ζ	permeability [m ²]	rev	reversible
r_{pore}	pore size of the porous media [m]	rib	rib in the interconnects
ε	porosity [-]		
A	pre-exponential factor ([S·K·m ⁻¹] for conductivity, [A·m ⁻²] for electrochemistry)	Superscripts	
		eff	effective
		0	standard

and sealing conditions [5]. In this regard, numerical simulations of the SOFC stacks using a high-fidelity physical model are essential techniques in understanding the thermo-fluid reacting environment and characterizing the local thermodynamic state in the vicinity of the cell [6].

To meet these needs, the high-fidelity physical models should be able to elucidate complex heat and mass transfer occurring within multi-dimensional SOFC stack structures. The SOFC stacks consist of the cells, each of which has a dense electrolyte and porous air and fuel electrodes, and metallic interconnects that connect the cells electronically and thermally with each other. At each unit-cell of the stacks, air and fuel domains are separated by the dense electrolyte through which oxygen ion conduction and heat conduction take place. In the porous electrodes, simultaneous thermal/mechanical solid-gas interactions and thermo-electrochemical reactions among surface and gas species occur. Their microstructure characterized by porosity, tortuosity and permeability makes the physical-chemical phenomena significantly complex. The metallic interconnects are in contact with the cells and gases enabling the flow of electronic current and heat transfer. To investigate these complicated environments, the physical models need to account for heterogeneous thermo-electrochemistry and

momentum/species/energy transport in the porous electrodes and through the electrolyte and interconnects. In addition, given this multi-dimensional stack structure, it is needed to resolve spatially the local thermodynamic state in order to elucidate the physical-chemical phenomena. Detailed spatial information obtained by using a three-dimensional model makes it possible to examine the effect of operating conditions such as fuel utilization on the thermo-fluid field and hence the heat and mass transfer.

Given these requirements, three-dimensional modeling studies for planar anode-supported SOFC stacks have been recently conducted. Table 1 summarizes representative SOFC modeling studies ranging from one-dimensional to three-dimensional approaches reported in the literature. Since three-dimensional SOFC models consider several solution variables and parameters and take into account fully-coupled nonlinear conservation equations as well as complex constitutive equations, they need significantly large computational resources to proceed simulations, which had limited SOFC numerical studies to lower dimensions [7–17]. One- or two-dimensional models were primarily used for developing electrochemical reaction mechanism and understanding cell operation mechanism, which is insufficient to elucidate phenomena occurring inside the multi-dimensional SOFC stacks. To tackle this issue,

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