Energy Conversion and Management 153 (2017) 175–187

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

Multi-scale multi-objective optimization and uncertainty analysis of methane-fed solid oxide fuel cells using Monte Carlo simulations

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ARTICLE INFO

Keywords:
Multi-objective
Solid oxide fuel cell
Direct internal reforming
Multi-scale
Monte Carlo simulation
Pareto

ABSTRACT

In this work, a multi-objective optimization approach is adopted for methane fueled solid oxide fuel cells in both microstructural and operational points of view. The optimization procedure was performed at different stages where microstructural parameters were considered separately and also in combination with operational variables in 2-objective and 3-objective cases. Effective reaction area, total conductivity and average pore radius are taken as the micro-model objective functions while system efficiency and power density as the multi-scale objectives are to be maximized. Electronic phase volume fraction, porosity, fuel utilization and steam/methane ratio are some of the important design parameters. The results of multi-objective problem are presented in terms of Pareto fronts of non-dominated solutions in which the compromised designs depicted among them. By multi-objective optimization of the microstructure of a solid oxide fuel cell anode, optimal electronic and ionic particle size of 0.4 and 0.26 μm, electronic volume fraction of 59% and porosity of 48% are determined. In addition, an optimum trade-off solution with 52% efficiency and 0.699 W/cm^2 power density is achieved by multi-scale multi-objective optimization of the system. Finally, an uncertainty analysis is implemented based on Monte Carlo simulations to show the statistical performance of system outputs as well as the probability of failure of system constraints.

1. Introduction

High temperature solid oxide fuel cells (SOFCs) have been identified as environmentally benign energy conversion device that have unique advantages such as high efficiency, high reaction kinetics and fuel flexibility. Despite recent theoretical and experimental progress in the theory of SOFCs, the technology still faces many challenges in a variety of aspects before it can evolve as a reliable energy production technology.

One of these aspects that remains lacking in the literature is the comprehensive performance optimization studies based on concurrent consideration of both microstructural and operational parameters of the system. The main prerequisite tool for optimization studies is mathematical models that can help us to understand complicated coupled phenomena within SOFCs. Several researchers investigated DIR SOFCs in different levels of complexity and from numerous aspects based on varying numerical and mathematical approaches. In this regard, T. X. Ho [1] presented a three dimensional dynamic numerical model of an anode-support DIR-SOFC subjected to unsteady condition. Tseronis et al. [2] developed a DIR-SOFC model without separate reformer using COMSOL software. Aguiar et al. [3] proposed and analyzed a quasi-two dimensional steady state mathematical model of an anode-support intermediate temperature DIR-SOFC at different co-flow and counter-flow operating conditions. Iwata et al. [4] presented a quasi-two dimensional co- and counter-flows model of planar SOFC. Janardhanan et al. [5] studied the differences in efficiency and power density for isothermal and adiabatic operational regimes of planar DIR-SOFCs. Ni et al. [6] worked on the performance of SOFCs running on methane fuel considering the effect of electrode structural. Albrecht and Braun [7] compared 1-D versus quasi 2-D models for predicting temperature gradient and species concentration within the anode gas channel along the cell length. In a subsequent study, Albrecht and Braun [8] benchmarked 1-D versus quasi 2-D dynamic, interface charge transport models in a comparison paper against other models.

Micro-scale models have also been extensively developed and studied based on different approaches. Image processing based 2D and 3D reconstruction models are widely used for microstructure design and optimization of SOFCs [9–11]. Celik et al. [9] developed micro-level

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http://dx.doi.org/10.1016/j.enconman.2017.10.011
Received 20 June 2017; Received in revised form 2 October 2017; Accepted 3 October 2017

Nomenclature

C	molar concentration (mol m^{-3})
D_i^{eff}	effective Fickian diffusivity of species i (m^2 s^{-1})
D_{ij}^{eff}	effective binary diffusivity (m^2 s^{-1})
$D_{i,k}^{eff}$	effective Knudsen diffusivity for species k (m^2 s^{-1})
F	Faraday's constant (96487 C mol^{-1})
j	operating current density (A m^{-2})
N	molar flux (mol m^{-2} s^{-1})
P	total pressure (Pa)
P_i	partial pressure of species i (Pa)
R	universal gas constant (8.314 J mol^{-1} K^{-1})
T	temperature (K)
y_i	mole fraction of species i
B_0	flow permeability (m^2)
L	channel length (m)
W	channel width (m)
Ar	aspect ratio of fuel or air channel
D_c	channel hydraulic diameter (m)
K^{eq}	equilibrium constant (Pa^2,–)
	pre-exponential constant (varies)
k	rate constants (varies)
Ref	product of the Reynolds number and friction factor
r	rate of reaction (mol m^{-2} s^{-1}, mol m^{-3} s^{-1})
t	thickness or height (m)
U	velocity (m s^{-1})
V_{cell}	cell voltage (V)
U_f	fuel utilization
X_{CH4}	methane conversion
S/M	steam to methane ratio
V_{OCV}	open circuit voltage (V)
$V_{leakage}$	leakage voltage (V)
$E_{act,i}$	activation energy of i electrode (J mol^{-1})
j_{TPB}	charge transfer rate per unit TPB length (A m^{-1})
$j_{0,i}$	local exchange transfer current per unit TPB length of i electrode (A m^{-1})
$J_{ref,i}$	current density at reference temperature (A m^{-1})
i_{ion}	local ionic current density (A m^{-2})
i_{el}	local electronic current density (A m^{-2})
$i_{e,i}^V$	volumetric charge transfer rate (A m^{-3})
M_α	molecular weight of species α (Kg mol^{-1})
n_k^V	number of k-particle per unit volume
P_k	percolation probability of k-particle
T_{ref}	reference temperature (K)
$Z_{k,l}$	average number of contacts between a k-particle and l-particle
$\widetilde{Z}$	overall average coordination number of all solid particles
LHV	lower heating value
$\dot{N}_f^0$	total molar flow rate of the fuel stream (mol s^{-1})
n_e	number of electrons participating in the electrochemical reaction
r_g	pore radius (m)

Greek

β	channel mass transfer coefficient (m s^{-1})
β_i	cathodic charge transfer coefficient of electrode i
α_i	anodic charge transfer coefficient of electrode i
η	overpotential (V)
ϕ	potential (V)
Θ	relative coverage
$\lambda_{TPB,eff}^V$	percolated TPB length per unit volume (m^2)
μ	dynamic viscosity (Kg m^{-1} s^{-1})
ϕ_g	porosity
ψ_k	volume fraction of k-particle in solid phase
ψ_k^t	threshold volume fraction of k-particles
σ_{ed}^{eff}	effective electronic conductivity (S m^{-1})
σ_{el}^{eff}	effective ionic conductivity (S m^{-1})
σ_k^0	electric conductivity of k-material in dense solid (S m^{-1})
τ	tortuosity of gas transport path
θ	contact angle between electrode- and electrolyte particles

Subscripts and superscripts

MSR	methane steam reforming reaction
WGS	water gas shift reaction
OX	electrochemical oxidation
sf	fuel species
sa	air species
TPB	triple phase boundary
act	activation
ohm	ohmic
k	reaction index
eff	effective
ref	reference
el	electrode-particle
ion	electrolyte-particle
t	total
A/C	anode channel interface
A/E	anode electrolyte interface
s	surface
a	anode
c	cathode

modeling of SOFCs for accurate estimation of real stresses for performance improvement. Hamedani et al. [10] characterized the microstructure of a porosity-graded cathode of SOFCs using ion beam and scanning electron microscopy. Taillon et al. [11] investigated the microstructure and connectivity of composite cathodes using dual beam focused ion beam in order to determine the effect of various contaminants on the performance of the SOFCs. Resistor network models are also investigated for microstructure analysis of SOFCs [12,13]. Jeon et al. [12] used a resistor network model for anodic performance enhancement by introducing penetrating electrolyte structure. Schneider et al. [13] deployed resistor network model to determine effective electrode conductivity based on a particle packing numerical approach. Electrode micro-models are also popular among researchers for optimization of electrode microstructure [14–16]. Nam and Jeon [14] developed a comprehensive micro-scale model for detailed description of micro-scale transport in SOFCs. Jeon et al. [15] optimized a two-layered cathode in anode-supported SOFCs based on a numerical micro-scale model. Ni et al. proposed mathematical model of functionally graded electrodes at the micro-scale level. Percolation based micro-models are simple and efficient for predicting effective properties of composite electrodes [17–19]. Chen et al. [17] suggested a percolation based micro-model which considered binary and multi-component mixtures of particles for predicting effective electrode properties. In another study, Chen et al. [18] developed a percolation micro-model to predict effective properties electrode consisting of poly-dispersed electronic and ionic conducting particles. Bertei and Nicolella [19] proposed a percolation model by accounting for polydispersion of powders and presence of pore formers.

Such micro-models are widely used in microstructural studies for optimization of porous SOFC electrodes [20,21] and in combination with macro-models for analyzing the effect of microstructural parameters on system output performance [22,23]. Liu et al. [20] offered a