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Degradation based operational optimization model to improve the productivity of energy systems, case study: Solid oxide fuel cell stacks

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ABSTRACT

In the present study a comprehensive thermodynamic model and degradation based optimization framework for energy management of anode supported solid oxide fuel cell (SOFC) stacks are carried out. The optimization framework determines optimum operating conditions to maximize system productivity (energy generation over system lifetime) considering degradation mechanisms. The main degradation mechanisms in anode supported SOFCs are nickel coarsening and oxidation. In this study, the optimum operating conditions regarding these degradation mechanisms to achieve maximum productivity at different target lifetimes are derived. The results show that target lifetime has a significant impact on system productivity and optimum operating temperature and current density. Furthermore, SOFC optimum operating conditions as a function of target lifetime are derived. To show the effectiveness of the developed framework, model outputs are compared with two other operating strategies; a base case strategy that optimizes system operating conditions without considering degradation mechanisms and a strategy based on Department of Energy's (DOE) 2016 fuel cell report. Results illustrated that degradation based optimization is more beneficial for improving the entire performance in long-term operation. For instance, system productivity is 7.4% higher in comparison with DOE strategy during 40,000 h operating lifetime. It is expected that the proposed methodology will lead to more rapid commercialization of SOFC technology.

1. Introduction

The solid oxide fuel cell (SOFC) is entirely solid-state and highly efficient. It has many advantages as a power generation device. For instance, it produces no noise during operation since it has no moving parts. In addition, the SOFC has no strict requirements on fuel gas composition. Unlike some other types of fuel cells that need pure hydrogen, the SOFC can use variety of fuels, most of which are hydrocarbon-based fuels such as methane and propane. The other advantage is that since SOFC operates at high temperatures, usually between 500 °C and 1000 °C, expensive platinum catalyst is not required. Also, the heat generated during operation can be used as a source of heat energy such as heating buildings [1]. However, due to issues caused by contaminants and degradation mechanisms over the long term, SOFCs are still not broadly implemented [2]. Thus, a fundamental understanding of degradation mechanisms for long term analysis of SOFC system is needed. Several studies have been conducted in recent years that model degradation mechanisms and the effect of degradation on performance deterioration [3–5]. For instance, in [6], a novel prediction approach for proton exchange membrane fuel cell performance deterioration is proposed based on a multi-physical aging model with particle filter approach. Optimizing operating conditions with considering performance deterioration leads to more accurate and reliable results [7,8].

In this study, a degradation based optimization (DBO) framework is proposed [9], and optimum operating conditions are derived in order to advance the commercialization of SOFCs.

Degradation based optimization is a model that accounts for system degradation mechanisms in the optimization procedure. The goal of the DBO is to derive the optimum operating conditions or design parameters of the system to maximize or minimize a specific objective function. In energy engineering systems, the optimum operating conditions mostly result in minimizing the system total cost or maximizing the system energy production through system operating lifetime [10,11].

There is a significant body of research that has focused on SOFC optimization models [12]. In most studies the optimization strategies are different. In addition, they are optimizing either operating

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Nomenclature

A	area, m^2
c_{O_2}	gas-phase concentration of O_2, mol m^{-3}
D	mass diffusivity, $m^2 s^{-1}$
E	activation energy, kJ mol^{-1}
F	Faraday's constant, C $equiv^{-1}$
H	enthalpy, J mol^{-1}
i	current density, A m^{-2}
I	working current, A
k_{ox}	rate constant for oxidation reaction, $m^3 kg^{-1} s^{-1}$
$k_{s,cap}$	nickel particles growth rate
L	length, m
M	molecular weight, kg mol^{-1}
n	equivalent electron per mole of reactant, equiv mol^{-1}
ni	number of nickel particles, mol
p	pressure, Pa
P	dimensionless pressure
pr	site occupation probability
R	universal gas constant, J $mol^{-1} K^{-1}$
r	nickel particles radius
r_{ox}	rate of oxidation, mol $kg^{-1} s^{-1}$
S^0	standard entropy, J $mol^{-1} K^{-1}$
T	temperature, K
TPB	triple phase boundary, m m^{-3}
u	decision variable
v	voltage, V
V_{Ni}	nickel particles volume
x	state variable
X	molar fraction of component in the mixture
β	Ohmic resistance, Ω
η	overpotential, V
σ	electrical conductivity, $\Omega^{-1} m^{-1}$
ϕ	porosity
ψ	tortuosity
ν	diffusion volume of simple molecules, cm^3
α	fraction of the reaction heat that is generated at the anode
δ	pre-exponential factor, $\Omega^{-1} m^{-2}$
θ_O	bulk oxygen coverage, dimensionless
γ	exponential activity parameter, kJ mol^{-1}
τ	perimeter

Subscript and super script

0	initial condition
1	bipolar plate (interconnect)
2	fuel channel
3	anode
4	electrolyte
5	cathode
6	air channel
Act	activation
ch	channel
Conc	concentration
Ohm	Ohmic
Opt	optimal
x	x direction
y	y direction
z	z direction

conditions or design parameters [13]. For instance, Feng et al. [14] developed a design optimization model to maximize system output power. In this study, the structure of a single tubular SOFC is considered as a decision variable. Results show that optimum structure leads system to operate at 18.2% higher output power in comparison with not-optimized structure design. Duhn et al. [15] proposed a novel optimization model to determine the optimal geometric flow design. The modeling of the system is based on the computational fluid dynamic modeling and decision variables are the channels width and the area in front of the parallel channels. The optimal design maximizes flow uniformity index which is directly proportional to the maximum obtainable overall conversion. Hasanabadi et al. [16] investigated a model to optimize the microstructure design of an SOFC. In their study two-point correlation functions are used to realize the three dimensional porous microstructure of the SOFC. The results show that the optimization procedure can be used as a robust tool to design the optimal microstructure.

In [17] a multi-objective optimization model is investigated that optimizes operating conditions of a tri-generation system driven by SOFC. In this study the objectives of the optimization are to minimize system total product unit cost and maximize exergy efficiency, simultaneously. The optimization algorithm is based on genetic algorithm and results indicate that optimal conditions are on the Pareto front. In [18], the operating conditions of a tri-generation system is optimized to make the system economically affordable while meeting the whole cooling demand and 50% of the total electricity demand. The model is optimized for a tri-generation system includes 50 kW tubular SOFC combined with heat recovery steam generator, combustion chamber and a chiller. Results show that optimal operating conditions lead system to be economically affordable and have an approximately net annual profit of $874,200.

The design parameters and operating conditions can be optimized more accurately by considering degradation mechanisms in the optimization procedure [19]. Xu et al. [20] developed an optimization model considering system degradation to optimize thermal stress performance of the SOFC. The aim of the model in their study is predicting the thermal stress of an anode-supported SOFC for different designs. A three dimensional thermal stress model is considered as the degradation mechanism. The results show that as the interconnect area increases, the thermal stress decreases. In addition, the thermal stress of the counter-flow and co-flow are similar.

As is clear from reviewed literature, most SOFC degradation models are based on experimental data. However, in principle-based models, the degradation mechanisms rate dependency to operating conditions and SOFC material properties can be determined more accurately.

As can be seen, in the case of SOFC optimization models, significant research has been done in the last decade [21–24]. However, there is not many studies that optimize system considering degradation [25–28]. The main contributions of the present study are as follow:

- One of the main novelties of the proposed framework is the consideration of degradation model in the optimization procedure. The degradation mechanism can result in performance system long term productivity deterioration. The rate of degradation mechanism depends on system operating conditions. Effective control of degradation mechanism rate is a key element of the efficient operation of energy systems. The proposed model manages degradation mechanism by optimizing system's operating conditions in order to maximize lifetime productivity.
- An improved degradation based optimization approach is used in order to address degradation mechanism effect on system productivity deterioration. This new approach results in more accuracy in long term simulation and more reliable and realistic optimal operating conditions.
- The proposed framework produces optimal operating conditions of SOFC stacks to achieve maximum productivity over system target