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Dimensional optimization of a tubular solid oxide fuel cell

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ABSTRACT

Solid oxide fuel cells (SOFCs) are very promising for their potential applications as power generators. However, the cost of these cells needs to be significantly reduced to make them a commercial success. Cost of the materials is a significant component of the overall cost. An improvement of the power density with respect to the weight of the cell, termed as gravimetric power density in this study, can help to achieve a lower material cost. On the other hand, a compact design is required for both man-portable and stationary powerhouse applications. The power density with respect to the overall volume of the cell is termed as volumetric power density in this study. A nonlinear constrained multiobjective optimization study using a lexicographic approach is performed to maximize the gravimetric and the volumetric power density of a tubular SOFC. The decision variables are the radius of the anode channel, the cell length, and the annulus size. To be used for optimization studies, a detailed steady state model is developed that can capture changes in the concentration, activation, and ohmic losses due to changes in the decision variables. The model is extensively validated with experimental data collected from an industrial cell spanning a wide range of temperatures, H_2 flow rates, and DC polarizations. Although the model predictions are found to be satisfactory for most operating conditions, a significant mismatch between the simulation results and the experimental data is observed when the H_2 flow rate is low. The validation study helps to identify the feasible region for the optimization study. The optimization study shows that significant improvements in both the power densities are possible for all the operating conditions considered in this study. The electrical efficiency of the cell also gets improved due to the optimization. In one of the operating conditions, about 30% improvement in the gravimetric power density and about 65% improvement in the volumetric power density are obtained due to the optimization. The percentage changes of the decision variables compared to their base case values are found to be similar for all the voltages other than the voltages close to the open circuit potential (OCP).

1. Introduction

Energy is the driving force of the modern civilization. The conversion efficiency of fuel to electric power is critical given that the fossil fuel sources are getting depleted rapidly. Fuel cells are envisaged as an effective technology to achieve high efficiency in this conversion process. SOFC is a high temperature fuel cell very suitable for combined cycle operation. In the future vision of the highly efficient power stations such as Integrated Gasification Combined Cycle (IGCC), SOFC is a key component (Williams, Strakey, & Sudoval, 2006).

With the focus on improvement of efficiency and cost, SOFC modeling studies need to capture the variables that affect the efficiency and cost of a SOFC. The dimensions of a SOFC, particularly that of a cylindrical cell, have a significant effect on the efficiency and cost of a cell. If the volume of the Positive Electrode–Electrolyte–Negative Electrode assembly (PEN) is kept constant, a decrease in the radius of the anode channel will result in a longer length of the cell. Again, if the total volume of the cell is constant for an anode-supported tubular SOFC, the change in the radius of the anode channel will result in a different size of the annulus of the cathode channel. As the cell length, the radius of the anode channel, and the annulus size of the cathode channel change, the pressure drop across the flow channels changes along with other transport fields. For a pressure driven flow, the maximum pressure is expected at the inlet of the gas channel. If a cell is run at the maximum pressure that the cell can withstand, then an increased pressure drop in the flow channels would result in an increase in the activation and concentration overpotentials of the cell. Also, the electrons have to flow from/to the current collectors to/from the TPB (Triple Phase Boundary, where the electrochemical reactions take place) because of the electrochemical reactions. As the current collectors are typically placed only over a small region

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Nomenclature

A_{act}	active area for electrochemical reactions, m^2
C	concentration of species, mol/m^3
D_{ac}	diameter of the anode channel, m
$D_{j,eff}$	effective diffusivity of species j, m^2/s
D_{j-n}	binary diffusion coefficient between species j and n, m^2/s
$D_{j,K,eff}$	effective Knudsen diffusivity for species j, m^2/s
E_{an}	activation energy for the anodic reaction, kJ/mol
E_{ca}	activation energy for the cathodic reaction, kJ/mol
F	Faraday's constant
I_i	current generated by the i th CV, A
k	pre-exponential factor, A/m^2
$r_{e,el}$	radius of the pores in electrodes, m
$r_{in,ac}$	inside radius of the anode channel, m
$r_{in,cc}$	inside radius of the cathode channel, m
$r_{out,cc}$	outside radius of the cathode channel, m
R_u	universal gas constant
R	ohmic resistance, Ω
u	axial velocity in the flow channel, m/s
v	radial velocity in the flow channel, m/s

Greek symbols

ε	porosity
ζ_{el}	tortuosity
α	transfer coefficient
η_{ohm}	polarization loss, v

Subscripts

ac	anode channel
an	anode
cc	cathode channel
ca	cathode
el	electrode (anode or cathode)
elec	electrolyte
i	index for the control volume
j	index for the species: H_2, O_2, N_2, H_2O

of the circumference, the current path length changes as the cell radius changes affecting the ohmic resistance of the cell. A change in the annulus size of the cathode channel affects the cathode activation and concentration polarizations which are significant for a tubular SOFC, especially at high current densities. Hence a decrease in the radius of the anode channel for an anode-supported tubular SOFC will increase the pressure drop in the anode channel because of the increased cell length and will decrease the ohmic resistance because of a shorter current path (assuming the thickness of the electrodes and electrolytes remains unchanged). This interplay suggests that the dimensions of the cell can be optimized for a given objective function (Bhattacharyya & Rengaswamy, 2009b). For dimensional optimization, a detailed model is necessary that can capture these changes.

Several steady state models of SOFC exist in the open literature. In order to precisely capture the change in the pressure drop inside the flow channels with changes in the cell dimensions, it is essential to include the momentum conservation equations in the model. However, the equation of motion is generally avoided in the modeling of SOFC (Bessette, Wepfer, & Winnick, 1995; Hussain, Li, & Dincer, 2006; Izzo, Perachhio, & Chiu, 2008; Jia, Jiang, Shen, & Abudula, 2008; Lim, Chadwick, & Kershenbaum, 2005; Ni, Leung, & Leung, 2007). The change in velocity, especially in the cathode gas flow channel, can be significant when the consumption of reactants is high in the cell (Bhattacharyya, Rengaswamy, & Caine, 2007). This can affect the cell performance particularly at higher current densities. Furthermore, the radial variation of the velocity and the concentration fields of the species can affect the cell performance. In the process of dimensional optimization, the cell radius is widely changed by the optimizer along with other dimensional variables (the decision variables). The models that do not consider the radial variation of the transport variables (Zhu & Kee, 2007) will not be able to capture the change in the cell performance (objective functions) during the optimization process.

One of the drawbacks of the tubular SOFC is the longer current path as compared to the planar SOFC (Bhattacharyya & Rengaswamy, 2009a). Because of the location of the current collectors, the movement of the electrons from/to the TPB to/from the current collectors can be characterized as a simultaneous circumferential and radial motion. In the optimization studies using this model, the thickness of the electrodes is not changed as the electrode thicknesses are chosen based on experimentation considering residual stress and mechanical integrity of the system. As the model developed in this study does not consider the stress developed in the solid part, no attempt is made to manipulate these variables. Even if the thickness of the electrodes is kept constant, a change in the radius changes the circumferential path length of the electrons and a change in the cell length change the cross-sectional area available for flow of electrons. The ohmic loss in the cell can be expressed as $\Delta E = IR$ where I is the current produced by the cell and R is the total ohmic resistance. Ohmic resistances of the electrodes and the electrolyte are often considered separately and expressed by $R_i = l_i\varphi_i/A_i$, where l, φ, and A are the corresponding length, resistivity, and area respectively. However, the length of current flow in the electrodes is difficult to determine because of the simultaneous flow of the electrons in both the circumferential and radial directions. The changed ohmic resistance because of the available paths for the flow of the electrons is generally not considered in the existing literature (Akkaya, 2007; Bessette et al., 1995; Campanari & Iora, 2004; Costamagna & Honegger, 1998; Izzo et al., 2008; Lim et al., 2005). If the dimensions of a cell are changed, these models will not be able to capture the changed resistances precisely and therefore are not a good choice for a model intended for optimization of the cell dimensions. A simple approach has been taken in this study by developing an equivalent circuit considering the ohmic resistances of the individual electrodes by a series and parallel combination of the resistances.

Several studies can be found where the SOFC model is not validated with the experimental data (Aguiar, Chadwick, & Kershenbaum, 2002; Campanari & Iora, 2004; Lim et al., 2005; Zhu & Khee, 2007). Validation studies for a single operating point can be found in some papers (Akkaya, 2007; Bessette et al., 1995; Hussain et al., 2006; Izzo et al., 2008; Jia et al., 2008). A good fit with the experimental data is often reported in a number of publications (Costamagna & Honegger, 1998; Leah, Brandon, & Aguiar, 2005; Mandin et al., 2006). However, the region in which the model is not valid often remains unidentified. Identification of this region is crucial for a model intended to be used for optimization studies because the feasible region for optimization should be the region in which the model is valid.

Optimization studies on SOFC are not many. However, based on the available literature, SOFC optimization can be classified into three broad categories—microstructural, unit level, and system level optimization. In microstructural optimization, grain size, mean pore diameter, thickness of the cathode functional layer, etc., are typically considered for optimization (Deseure, Bultel, Dessemond, & Siebert, 2005; Jeon, Nam, & Kim, 2006). At system level optimization, different configurations, combination with different equipments ,and optimum operating conditions are explored (Baratto & Diwekar, 2005; Calise, Accadia, Vanoli,