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Reduced non-isothermal model for the planar solid oxide fuel cell and stack

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ABSTRACT

The combination of spatial smoothing and asymptotic analysis allows reduction of computationally expensive 3D fuel cell models to 2D without sacrificing leading-order physics. This paper investigates, demonstrates, and verifies the spatial smoothing and asymptotic reduction of a 3D non-isothermal model for the planar solid oxide fuel cell and stack. Particularly, spatially-smoothed energy equations are developed subject to LTE (local thermal equilibrium) and LTNE (local thermal non-equilibrium) conditions in the flow field consisting of parallel plain channels and solid ribs. The selection of either the LTE or LTNE set for use depends on the temperature difference between the gas flow in channels and the ribs. The reduced models agree well with the 3D counterpart in view of the quantified loss of information due to reduction, while the computational cost is reduced by more than three orders of magnitude. The present methodology is generic and can be applied to other types of fuel cells which are slender in shape and equipped with parallel channels. The reduced model allows statistical sensitivity analysis of cell/stack performance with respect to modeling parameters in a large sample size at computational cost that is not prohibitive.

1. Introduction

The SOFC (solid oxide fuel cell) operates at high temperatures ranging from 500 to 1000 °C [1–5]. During operation, heat is generated via the electrochemical reactions within the reaction zones and the current passing through the cell. The heat transfer in the solid structures occurs mainly through conduction, while convective heat transfer dominates in the gas channels and the pores of electrodes. In order to investigate the multiphysical behaviors of the SOFC, mathematical modeling is an efficient approach compared with experimental techniques. An isothermal condition is usually applicable for single-cell modeling when the cell behaves isothermally at the leading order [6–8], whereas the temperature of a SOFC in a stack may undergo leading-order changes [9]. Large temperature gradients in the SOFC stack can cause undesired large thermal–mechanical stresses and thermal expansion mismatches, since the SOFC generally consists of ceramic components with different thermal expansion coefficients [10,11]. This may thus result in the thermal–mechanical degradation and/or structure failure of the SOFC. Moreover, the material properties of the SOFC are strong functions of temperature, and the reaction rates of the electrochemical reactions are temperature-dependent as well [12]. Therefore, efficient and reliable non-isothermal models that can provide accurate prediction of the temperature distribution are essential for designing and optimizing the SOFC stack.

A non-isothermal SOFC model is generally expressed in the form of elliptic PDEs (partial differential equations) for the conservation of mass, momentum, species, charge, and energy coupled with relevant constitutive relations and boundary conditions [12–14]; radiation is generally neglected [1,12,15–18]. The energy transport in the SOFCs can be modeled either in a LTE (local thermal equilibrium) or LTNE (local thermal non-equilibrium) approach [13]. LTE prescribes the same temperature for the gas and solid phases associated with effective transport parameters based on volume-averaging for porous media [12,19–24], whereas LTNE predicts the temperatures of the solid and gas phases within the porous media separately, namely T_s and T_g [17,25,26]. Zheng et al. [27] proved that the difference between the solid and gas phases in the porous electrode is insignificant for the SOFC and it's safe to apply LTE to SOFC modeling.

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Detailed 3D (three-dimensional) SOFC models are computationally expensive – both in terms of computational time and memory requirements – due to not only the highly coupled and nonlinear nature of the mathematical formulation but also the large number of functional domains including interconnects, flow channels, backing layers, reaction zone layers, and an electrolyte in each cell of the stack. Two common assumptions are usually made to reduce the complexity of modeling for the SOFC: simplifying the model dimensionality from 3D to two (2D) [21,28–31], one (1D) [32–34], or zero dimension (0D) [35,36]; and reducing the reaction zone from a spatial domain [8,10,37–43] to a boundary or interface condition [9,16,21,24,28,29,33,36,44–51]. However, these assumptions are likely to lower the fidelity of the model predictions. These simplified models do not account for the influence of ribs on the thermo-fluid mechanics in the flow field or the pathways of transport processes from the flow field to its adjacent layers that may cause depletion of reactions at positions in the electrode under the ribs. Moreover, dependent variables can undergo spatial changes in the reaction zones [8,37–42].

Apart from assuming a lower dimensionality instead of 3D for modeling, reducing the formulations and/or geometry of a fuel cell model is another way to alleviate the model complexity and computational cost. Iwai et al. [17] and Roos et al. [52] applied the volume-averaging theory for the SOFC to reduce a 3D flow field of channels separated by ribs to a 2D porous counterpart, such that the normal direction ($\mathbf{e}_z$ in Fig. 1) in the flow field was omitted from the model. However, they did not formulate the effective transport parameters for the porous flow field counterpart in terms of the geometrical properties of the channels and ribs in the 3D flow field. They specified constant values for the effective parameters for the porous flow field counterpart, but did not justify the validity of the specified constant properties for different geometrical designs of the channels and ribs. The effect of the ribs on the pathways of transport processes between the flow field and adjacent layers were not taken into account. In addition, neither Iwai et al. [17] nor Roos et al. [52] compared the reduced P-SOFC (planar SOFC) model with the original 3D counterpart to justify that the reduced formulations can capture the leading-order physics of the full 3D model. In order to reduce the model without sacrificing the leading-order physics, we investigated spatial smoothing based on volume-averaging over a flow field comprising parallel channels separated by ribs for the PEMFC (proton exchange membrane fuel cell) [53] and the P-SOFC (planar SOFC) [54], respectively. Via the spatial smoothing followed by asymptotic reduction, the 3D model in the form of elliptic PDEs was reduced to a 2D counterpart that consisted of parabolic PDEs and ODEs (ordinary differential equations) associated with a space-marching algorithm. Effective transport properties and correlation factors that were expressed in terms of the geometrical parameters of the cell were developed and introduced to the transport equations to account for the mechanics in the neglected spanwise direction ($\mathbf{e}_y$ in Fig. 1) in the flow field and the influence of ribs on the pathways of mass and charge transports. Good agreement was obtained for the verification of the spatially-smoothed models and their asymptotic counterparts with respect to the 3D models. Nevertheless, the studies in Refs. [53,54] were conducted under an isothermal condition for single-cell modeling. The spatial smoothing for non-isothermal fuel cell models has not been studied in the literature.

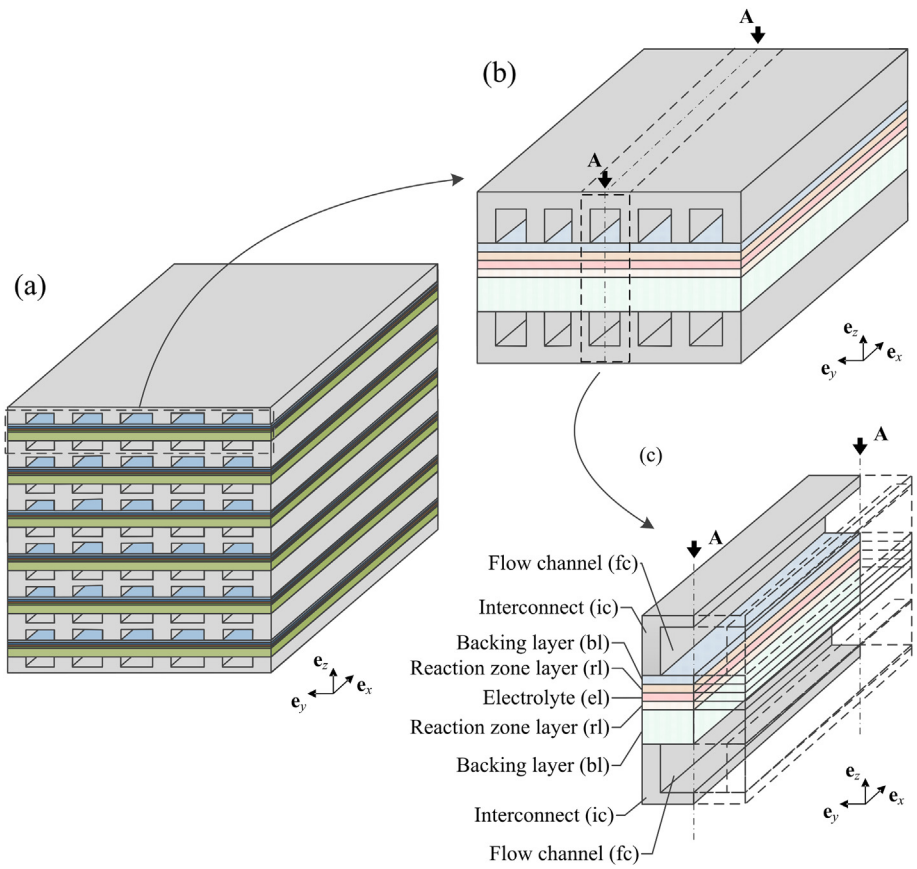

Fig. 1. Schematic of (a) a P-SOFC stack with parallel plain channels, (b) a 3D single cell, (c) a repeating unit with a pair of channels.

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