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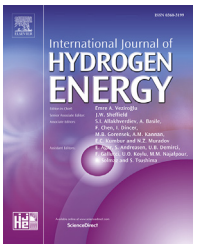

3D and simplified pseudo-2D modeling of single cell of a high temperature solid oxide fuel cell to be used for online control strategies

Babak Ghorbani, Krishna Vijayaraghavan *

School of Mechatronic Systems Engineering, Simon Fraser University, 250-13450 102 Avenue, Surrey, BC, V3T 0A3, Canada

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ABSTRACT

In the current study, a single cell of a planar SOFC is firstly modeled in 3D using commercial SOFC module of ANSYS Fluent and the results are validated against the experimental investigations in the literature. Many researchers have used ANSYS Fluent for simulating solid oxide fuel cells. However, there is a huge gap in the literature on explaining the detailed procedure that should be followed in order to use this software effectively. A thorough step-by-step approach is presented to provide a deep insight into the software. Thereafter, a simplified quasi-2D method with infinitely shorter computational time is developed and the results are compared with the 3D model. It is found that the reduced model is capable of being utilized as an alternate method for both online diagnosis and designing active control strategies.

Introduction

Reducing the fossil fuel consumption at a rapid due to rising issues make the emergence of green power market necessary [1]. Among all green technologies, fuel cells transfer the chemical energy directly into electricity without combustion [2]. Fuel cells are thus not limited by the Carnot cycle efficiency and can produce electricity at very high efficiencies. They are recognized as one of the most promising environmentally-friendly technologies for producing electricity. Fuel cells are classified into proton exchange membrane fuel cells (PEMFCs) and solid oxide fuel cells (SOFCs) [3] based on their electrolyte material. SOFCs operate between 500 and 1000 °C and use ceramic electrolytes. As a result, SOFCs have higher power densities [4] and efficiency [5], offer fuel flexibility [6] modularity [7] and the ability of utilization for cogeneration [8], use of less expensive catalyst material [9], and have much longer lifetimes [10]. Modeling of SOFCs enables an inexpensive method to analyze the performance of SOFCs [11] as well as to develop controllers [12,13]. SOFC dynamics are highly nonlinear, and models for online control strategies need to be computationally efficient [12] and balance accuracy with speed [13]. Such high fidelity, computationally efficient SOFC models will also enable diagnosing faults (such as chromium poisoning) and would greatly aid in the expanded adoption of SOFC.

* *Corresponding author.*
E-mail address: krishna@sfu.ca (K. Vijayaraghavan).

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Models that aim to capture all the underlying interactions between the various physical phenomena in the fuel cell are known as full physics simulations. Full physics simulations take into account the coupled mass, momentum, energy, species, and charge transfer equations along with the corresponding boundary conditions [14–16]. Full physics three-dimensional (3D) models using the finite volume approach [17] are capable of capturing the internal dynamics of the SOFCs with relatively high accuracy. Three-dimensional models have been used in literature in design optimization and in modeling fuel cell stacks [18–22]. Among these, the most often cited model presented by Achenbach [22] is capable of simultaneously solving mass, momentum, energy and electrochemistry equations. The model also offers co-flow, counter-flow, and cross-flow configurations.

Full physics 3D models require significant computations [23]. There are two main approaches to reduce the amount of computation required. The first set of methodologies involve simplifying the 3D model into either 2D models [24–26], 1D models [12,27,28], or lumped parameter 0D models [29]. The second set of methodologies involve lowering the computational burden by modeling the electrochemical reactions at the triple phase boundary of the electrolyte, as a voltage jump at an interface [18,19,21,24,25,27,30–32]. The second approach has been well studied and most researchers have used ANSYS Fluent, a commercial CFD software, for their simulations. The first approach (reduced dimension) offers faster convergence at the expense of reduced modeling accuracy. Among all, 0D models, which are sometimes referred to as black box models, are the simplest methods. 0D models are categorized as either empirical models (where experimental tests are conducted for studying the performance of the fuel cell) [33], or "state of the art" models (when the fuel cell is only treated as a component of an energy conversion system) [34]. 1D models only take one geometrical dimension into account which is mostly same as flow direction. 1D models are flexible to be utilized for both planar [35] and tubular [36–38] fuel cells. Basically, 0D and 1D models must be utilized only when no information about the fuel cell itself is required [13] since they are based on so many simplifying assumptions. 2D models neglect only one physical dimension so they yield the closest results to full physics 3D methods. However, they still suffer from computational burdens unless more simplifying physical assumptions are made. Generally speaking, 2D models are more effective for tubular SOFCs in comparison with planar SOFCs as they do not cause any loss of information, thanks to circular symmetry of the cell [39]. Despite its improved computational efficiency over the full physics simulations, the second approach (reduced physics) still requires a significant amount of time to converge and the method is still unsuitable for online control.

It is possible to combine reduced dimension and reduced physics methods in order to achieve novel, effective, and efficient solutions. Models built using this approach are called multi-dimensional models [39]. Goldin et al. [40] introduced a new algorithm to couple CFD in Fluent with full chemical kinetics in a tubular SOFC by utilizing *user-defined functions* (UDF) in Fluent. The Fluent-UDFs recognize axis of a tube, creating a unit axis vector in the direction of the tube. 1D band mesh is then applied to the surface of the tube and the chemical kinetics within the tube are calculated in 1D. These results are subsequently (iteratively) mapped to the 3D mesh. Kattke et al. [41] used this coupling algorithm for stack and system design of tubular SOFC followed by thermal management of the stack. Finally, Kattke and Braun [42] utilized their previous work [41] in a steady state analysis to find important control variables, identify operating strategies, and perceive how system design parameters (such as surface spectral properties and insulation) affect the system performance. Their model is also capable of understanding the thermal interaction between components of the fuel cell stack itself as well as their interactions with the surrounding. All studies mentioned here [40–42] combined the so-called reduced physics and reduced dimension in a novel way. However, their work is limited to tubular SOFCs and still needs long computational times as part of the domain is still modeled in 3D.

The main objective of this study is to improve modeling computation efficiency by coupling reduced dimension and reduced physics models, developing the pseudo-2D approach. The proposed model is an adaptation of a pseudo-2D model for PEM fuel cells and aims to combine the computational efficiencies of simplified models with the accuracy of full physics CFD simulations. The paper first presents a full physics 3D simulation of the SOFC that is then used for comparing the results. All CFD simulations in general, and simplified models in particular, need to be validated against real experimental results to ensure the accuracy [26]. For this purpose, it is a vital task to run the simulation using 3D and simplified models and to validate both models against the experimental data presented in the literature. ANSYS Fluent has been utilized in the current study in order to solve the mass, momentum, energy, species, and charge transfer equations in 3D simultaneously. Numerous software-based studies can be found in the literature, modeling SOFCs' performance using either ANSYS Fluent [43–59] or COMSOL Multiphysics [60–70]. Although there are several previous studies that have developed user-defined functions to be utilized along with the ANSYS Fluent, and few other studies which used the SOFC module of ANSYS Fluent directly, none of them provide a detailed step-by-step procedure required to help the simulations converge efficiently. Such information is crucial to ensure the convergence of commercial CFD simulations. Hence, a step-by-step approach followed by details on all effective parameters such as all boundary conditions, solution methods, material properties, thermo-physical properties, electrochemical parameters, meshing, solution controls, and appropriate solver settings will be represented in order to provide the reader with a deep insight into the software. Thereafter, the simplified pseudo-2D model has been developed for simulating the SOFC to show if it can produce the same accuracy as a full 3D simulation.

Numerical modeling

The following section summarizes the partial differential equations used to model the physics in a fuel cell. Schematic of the 3D model is depicted in Fig. 1. Hydrogen enters the anode section at the beginning of the channel whereas Air is fed to the cathode on the other side to account for the counter-flow configuration. Both air and fuel then diffuse along the

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