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Transient dynamic and modeling parameter sensitivity analysis of 1D solid oxide fuel cell model

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ABSTRACT

In this paper, a multiphysics solid oxide fuel cell (SOFC) dynamic model is developed by using a one dimensional (1D) modeling approach. The dynamic effects of double layer capacitance on the electrochemical domain and the dynamic effect of thermal capacity on thermal domain are thoroughly considered. The 1D approach allows the model to predict the non-uniform distributions of current density, gas pressure and temperature in SOFC during its operation. The developed model has been experimentally validated, under different conditions of temperature and gas pressure. Based on the proposed model, the explicit time constant expressions for different dynamic phenomena in SOFC have been given and discussed in detail. A parameters sensitivity study has also been performed and discussed by using statistical Multi Parameter Sensitivity Analysis (MPSA) method, in order to investigate the impact of parameters on the modeling accuracy.

1. Introduction

Solid oxide fuel cell (SOFC) is considered as one of potential candidates for the renewable energy applications in the future. The SOFC based energy production systems are well known for their high energy efficiency, environmentally friendly by-products and wide power range (from some kW to some MW) in different applications. The SOFC uses solid ceramic materials (usually YSZ, Yttria-Stabilized Zirconia) as electrolyte, to operate at very high temperature (typically 700–1000 °C). The structures of SOFC can be mainly distinguished into two types: tubular SOFC structure and planar SOFC structure. During the operation of an anode supported tubular SOFC, hydrogen is supplied to the inner tube of cell (e.g. anode) and air is supplied to the outer surface of cell (e.g. cathode). The reactant gases diffuse through a porous ceramic electrode to reach the catalytic zone (usually Ni is used as catalyst). At the cathode, oxygen is reduced to oxygen–ion (O^{2-}). At the anode, hydrogen is oxidized to proton (H^{+}). The oxygen–ion passes through the solid electrolyte and forms water with the proton at the anode. The ceramic electrolyte is impermeable to electrons. Thus, the electron takes the path of external circuit from anode to cathode, supplying electrical power to an external load.

The SOFC operation involves some complicate multiphysics phenomena, including electrochemical reactions, gas diffusions and heat generations. In order to explain the operation characteristics and predict its performance, an accurate mathematical model needs to be developed. However, due to the complexity of physical phenomena in SOFC as well as the lack of details about the used materials, some empirical parameters are usually used in SOFC models. The choice of the numeric values of these empirical parameters may significantly impacts the accuracy of the developed model. Thus, performing the parameters sensitivity analysis is required for providing a reliable model. Such analysis could reveal the different degrees of sensitivity of the parameters in a model. The analysis results could be used as references for determining empirical parameters from experimental tests.

Furthermore, SOFC transient behaviors could be observed during the load power variations. The dynamic behaviors of SOFC have a direct impact on the fuel cell system component design, for example, the design of the power converter connected to the fuel cells. A better understanding of the dynamic behaviors in a fuel cell could facilitate the design and conditioning of the system.

In the literature, an electrical model that includes simple thermal dynamic for a 5-cells SOFC stack with experimental validations has been given in [1]. The proposed model has been used to investigate the temperature and output voltage variation between different cells in the stack. Only the large time scale dynamic (up to

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some hours) has been considered in the model. A simple 0D SOFC model that focuses on the influence of cell heat capacity on the thermal dynamic response has been presented in [2]. The large time scale dynamic response of the cell temperature and voltage due to the cell current change has been discussed in detail. A more detailed planar SOFC electrochemical model has been introduced in [3]. The model takes into account the hydrogen consumption across the gas channels. A power density analysis in SOFC has also been given for different cell geometries. However, the thermal dynamic has not been included in the model. A 1D tubular SOFC model has been developed in [4]. The model considers the local current density and a prediction accuracy comparison between 0D and 1D model has been made. Furthermore, the thermal modeling has been considered in a SOFC-micro gas turbine hybrid power system model in [5]. The model has been developed by using a least squares support vector machine (LS-SVM) identification method. Even though the thermal responses can be successfully predicted by the proposed modeling method, the mathematical fitting-model does not include any physical thermal phenomena equation. A simple physical SOFC model coupled with a micro gas turbine has been introduced in [6], however the presented model takes into account only the electrochemical phenomena. A similar simple electrochemical SOFC model has also been reported in [7], as a part of a fuel cell powered vehicle system model. A parametric study of a SOFC electrochemical model has been presented in [8]. The influence of the cell geometric and operating parameters on the SOFC performance has been discussed in great detail. however, the thermal domain has not been modeled. in addition to single cell modeling, The 1D IP-SOFC stack model presented in [9] demonstrates the non-uniform effect of SOFC parameters in the case of a 15 cells stack. A more complete model for a combined fuel reforming and SOFC system has been developed in [10]. The energy efficiency of such a system has been studied. A planar SOFC 2D model has been developed in [11] in COMSOL modeling environment. A dusty-gas model has been used to model the diffusion phenomena in the SOFC electrodes. The non-isothermal effect has also been considered. However, the model in [11] has been experimentally validated only for one operating condition at the steady-state. Another steady-state planar SOFC 2D stack model has been proposed in [12] with a model reduction method. The model predicted the current density and temperature distribution in the planar SOFC under steady-state conditions has been discussed. A 2D SOFC which covers electrochemical, thermal and fluidic domains has been presented in [13], with an investigation of cell operating parameters, such as inlet gas composition and electrode porosity. In [14], a 2D SOFC model with the consideration of partially pre-reformed inlet gas has been introduced. The cell performance has been evaluated by considering internal reforming process and water gas shift phenomena. Some other 2D SOFC models can also be found in the literature for cell performance prediction and fuel composition investigation [15–17]. A detailed 3D computational fluid dynamic model for a planar SOFC has been introduced in [18] for optimization purpose. Although the 3-D model shows a great interest for SOFC design improvement, the complexity of a 3-D model could limit its use in different applications. An investigation of the electrode thickness on the SOFC performance has also been made by proposing a two finite layers model of SOFC electrode in [19]. The modeling focuses are only made on the electrochemical phenomena in the SOFC. A 3D multiphysics model for a planar SOFC has been reported in [20]. The temperature and current density distributions of four different flow fields have been shown and discussed. A study in the effects of radiative heat transfer of SOFC has been introduced in [21] by using a detailed finite volume SOFC model with internal gas reforming. The factors that can lead to a decrease of SOFC efficiency have been discussed. In [22], the thermal time constant for SOFC has been investigated and discussed. The results show that the thermal processes of the fuel cell is the most important in modeling systems due to their influence on other parameters. Similar conclusion can also be found in [23] for a micro-tubular SOFC. In addition, SOFC material and geometry studies for the dynamic operation have also been presented in [24]. Based on a steady-state finite volume SOFC model, the influence of operating parameters on the SOFC performance has been discussed in [25]. The influence of the finite volume section number on the model output has also been shown. A sensitivity analysis for the geometry parameters of a planar SOFC using a 3-D model and a discrete adjoint method has been presented in [26]. An electrochemical parameter sensitivity analysis has also been introduced in [27] and [28] for low temperature proton exchange membrane fuel cells (PEMFC). The results show that, the electrode activation-related parameters have the most impact on PEMFC performance.

In this paper, a dynamic multiphysics model of a tubular solid oxide fuel cell is presented by using one dimensional modeling approach. The model is validated experimentally in different operating conditions. The non-uniformity effect, such as current density distribution, has also been shown and discussed. The fuel cell dynamic effects due to the double layer capacitances and cell thermal capacity are discussed later. The first order time constant expression for each dynamic phenomenon is calculated and discussed in detail. At last, a modeling parameters sensitivity analysis is performed for different semi-empirical parameters used in the SOFC model. The different degrees of sensitivity for semi-empirical parameters are shown and carefully discussed.

The main objectives of this paper are then: (1) Providing a dynamic, multiphysics 1D tubular SOFC model with experimental validations; (2) Discussing the dynamic phenomena in SOFC and giving the mathematical estimations of dynamic transient time; (3) Performing modeling parameters sensitivity analysis in different physical domains to show the different influences of parameters on the SOFC model output. The remainder of the paper is organized as follows. The next section presents in detail the proposed mathematical dynamic model for an anode supported high temperature tubular SOFC. The third section experimentally validates the 1D multiphysics SOFC dynamic model through an SOFC prototype. In the fourth section, the dynamic phenomena are investigated in detail in electrochemical and thermal domains. The last section gives a detailed parameters sensitivity analysis for semi-empirical parameters in the SOFC model, before concluding.

2. Solid–oxide fuel cell modeling

The multiphysics model presented in this section considers electrochemical, fluidic and thermal domains. Besides, the model includes electrochemical and thermal dynamic phenomena. The electrochemical dynamic phenomenon is due to the double layer capacitances, whereas the thermal dynamic phenomenon is due to the cell thermal capacity. The governing equations of the model are presented hereafter.

2.1. Electrochemical domain governing equations

The SOFC output voltage can be described by the following equation:

$$V_{cell} = E_{EMF} - V_{act,C} - V_{act,A} - V_{ohm} \quad (1)$$

where E_{EMF} is the cell thermodynamic voltage (V), V_{ohm} is the cell ohmic losses (V) and $V_{act,C}$, $V_{act,A}$ are the cell activation losses (V) of the cathode and the anode side, respectively.