



Research Paper

Numerical simulation of cell-to-cell performance variation within a syngas-fuelled planar solid oxide fuel cell stack

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HIGHLIGHTS

- Comprehensive 3D SOFC stack model.
- Quantitative index for cell-to-cell non-uniformity.
- Regularity of cell voltage variation in a stack.
- Cell voltage characteristic diagram of SOFC stack.
- Stack performance non-uniformity in different working conditions.

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ABSTRACT

The cell-to-cell voltage variation in a planar solid oxide fuel cell (SOFC) stack is numerically investigated, considering the coupling effect of the heat transfer and uniform mass flow rate distribution between cells. The model integrates validated three-dimensional electro-chemical button cell sub-models with the structure of a real counter-flow planar SOFC stack. A uniform characteristic diagram is defined to analyse the variation of the cell voltage distribution in a planar SOFC stack. A quantitative index of uniformity is proposed to compare and explain the difference in the cell voltage distribution uniformity in planar SOFC stacks. The simulation results indicate that the distribution characteristics of the cell voltage within a planar SOFC stack are primarily determined by the combined effects of the mass flow rate distribution and temperature distribution. The mass flow rate distribution dominates the overall cell voltage distribution trend, and the temperature distribution mainly dominates the cell voltage distribution of the cell near the top and bottom of the stack due to the thermal effects. The simulation results also indicate the relative uniform cell voltage distribution in planar SOFC stacks in the case of using syngas as a fuel instead of hydrogen.

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1. Introduction

A solid oxide fuel cell (SOFC) is an electrochemical device with solid oxide as an electrolyte and can convert fuel chemical energy directly into electricity [1]. Planar SOFCs are paid the most attention to due to their higher efficiency and lower material cost [2]. To obtain a higher power output for practical application, single cells are piled up in series to provide a higher working voltage. However, experimental studies [3,4] revealed that the cell voltage difference among cells in a stack can lead to long-run structural problems and eventually to stack failure [5].

Cell voltage variation among cells in a SOFC stack can result from asymmetry characteristics within the stack, for example, a non-uniform gas distribution in the stacking direction [6]. In a SOFC stack, a manifold is applied to connect the gas channels of the cells in parallel to distribute the fuel and air into each cell. Costamagna et al. [7] conducted one of the first numerical studies on the velocity distribution uniformity among cells in a fuel cell stack, considering the shape factors of the manifold. Boersma et al. [8] described the effect of the manifold shape and electro-chemical reaction on the gas flow by flow resistance and developed a network model to predict the gas distribution. Koh et al. [9] developed a systematic algorithm to calculate the pressure losses from different origins and predict the gas distribution. Kee et al. [10] proposed a generalized 2D CFD model to predict the gas distribution in a Z-type manifold. Bi et al. [11] performed a 3D CFD

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calculation for planar SOFC stacks with real stack geometry and found that the flow distribution is more uniform for a larger stack.

On the other hand, the temperature distribution within the stack due to the thermal effect can result in cell voltage variations even when the gas distribution is uniform [12]. Burt et al. [5] developed a pseudo-2D model to investigate the cell voltage variation in an SOFC stack, considering the effects of the gas distribution and temperature distribution. The result indicated that the cell voltage variations were influenced by the asymmetry that results from the uniform gas distribution and temperature uniformity. The cell voltage can vary by 12.3% due to the less uniform fuel distribution. Yuan [13] developed a pseudo-3D model to investigate the effects of heat transfer and uniform gas distribution in the stacking direction. The results showed that the selected uniform fuel distribution can lead to a 13% cell voltage variation in the stack.

In order to obtain the full insight of the cell voltage variation among cells within a planar SOFC stack, the effect of the flow distribution and the temperature distribution have to be fully considered. A SOFC stack model fully considering the effects of heat transfer and the detailed manifold geometry is needed. In this paper, a full 3D mechanistic model of a planar SOFC stack is developed considering the detailed transport processes of mass, momentum, heat and charge, as well as the chemical/electrochemical reactions [14] to predict the cell voltage variation within a planar SOFC stack. Instead of giving a certain gas distribution, a manifold is applied to simulate the gas distribution in a stack in practical development procedures. A validated electrochemical model is coupled with heat and momentum transfer to simulate a SOFC cell unit. Then, a SOFC stack model is developed by connecting SOFC cells in series. The non-uniform distributions of the mass flow rate, temperature and cell voltage is observed. By comparing to the base case, a SOFC stack without thermal effect and a SOFC stack with uniform gas distribution, a possible regularity of the cell voltage variation among cells in a stack is proposed [14]. A distribution characteristic is defined to analyse the cell voltage within a planar SOFC stack. The distribution characteristic and uniformity index and the effects of other factors, such as cell number in a stack and fuel components, on the cell voltage distribution were also analysed.

2. Model development

2.1. Geometry and mesh

A sketch of a typical planar SOFC unit is shown in Fig. 1. The main parameters of the planar SOFC unit are listed in Table 1. The mesh is set based on the simulation works from Wang et al. [15]

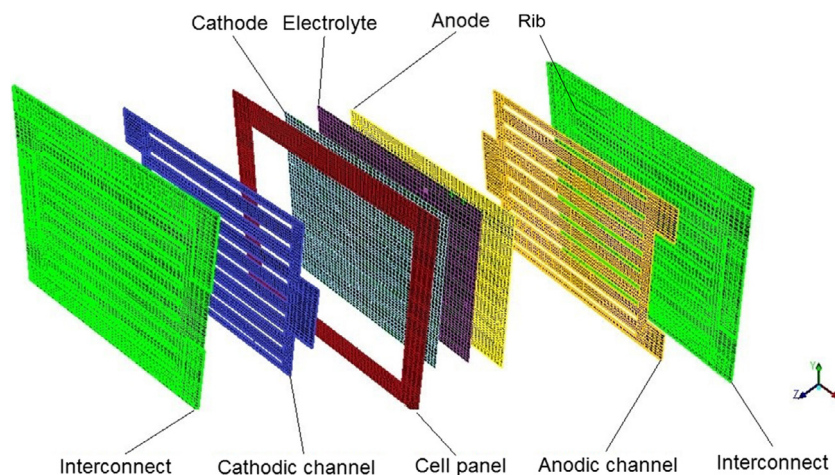


Fig. 1. Sketch of a planar SOFC unit.

To simulate a SOFC stack, the gas channels of each cell unit are connected in parallel by the manifold. As seen from Fig. 2, a Z-type gas supply scheme is applied in the study. A sketch of the manifold structure is shown in Fig. 3. The key parameters of the manifold are listed in Table 2.

2.2. Model assumptions

The main assumptions for the stack simulation include:

- (1) The model is set at steady state.
- (2) Every gas mixture is assumed as ideal gas.
- (3) The chemical and electrochemical reaction active sites are assumed uniformly distributed within the porous electrode.
- (4) Thermal boundary conditions of the stack outer faces are isothermal.
- (5) Radiation heat transfer within the SOFC stack is neglected.

2.3. Governing equations

The commercial CFD software Fluent™ is applied, and the electrochemical behaviour is described by the self-developed sub-routines. The electrochemical model is validated by experimental data and then combined with heat and mass transfer to form a SOFC unit model. The SOFC unit models are then integrated to be a SOFC stack model.

2.3.1. Charge balance

The charge balance governing equations are summarized in Table 3.

Where S_{TPB} is the volumetric triple phase boundary (TPB) area ($\text{m}^2 \cdot \text{m}^{-3}$) [16–19]

$$S_{act} = \pi \sin^2 \theta r_{elec}^2 N_{tot} n_{elec} n_{ion} \frac{Z_{elec} Z_{ion}}{Z} P_{elec-elec} P_{ion-ion} \quad (1)$$

where θ is the contact angle between the ionic and electronic conducting particles, which is set at 15° in this paper [17]. r_{elec} is the radius of the electronic conducting particles. N_{tot} is the total number of the electronic and ionic conducting particles per unit volume, which is formulated as

$$N_{tot} = \frac{1 - \varepsilon}{(4/3)\pi r_{elec}^3 [n_{elec} + (1 - n_{elec})(r_{ion}/r_{elec})^3]} \quad (2)$$

r_{ion} is the radius of the ionic conducting particles. n_{elec} and n_{ion} are the fractions of electronic and ionic conducting particles, respec-

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