Three dimensional CFD modeling and experimental validation of a single chamber solid oxide fuel cell fed by methane

H T Nguyen¹, M V Le¹, T A Nguyen¹, T A N Nguyen²

¹ Faculty of Chemical Engineering, Ho Chi Minh City University of Technology, District 10, Ho Chi Minh City, Vietnam
² Faculty of Applied Science, Ton Duc Thang University, 19 Nguyen Huu Tho Str., District 7, Ho Chi Minh City, Vietnam

E-mail: anh.nguyen@hcmut.edu.vn, lmvien@hcmut.edu.vn

Abstract. The solid oxide fuel cell is one of the promising technologies for future energy demand. Solid oxide fuel cell operated in the single-chamber mode exhibits several advantages over conventional single oxide fuel cell due to the simplified, compact, sealing-free cell structure. There are some studies on simulating the behavior of this type of fuel cell but they mainly focus on the 2D model. In the present study, a three-dimensional numerical model of a single chamber solid oxide fuel cell (SOFC) is reported and solved using COMSOL Multiphysics software. Experiments of a planar button solid oxide fuel cell were used to verify the simulation results. The system is fed by methane and oxygen and operated at 700 °C. The cathode is LSCF6482, the anode is GDC-Ni, the electrolyte is LDM and the operating pressure is 1 atm. There was a good agreement between the cell temperature and current voltage estimated from the model and measured from the experiment. The results indicate that the model is applicable for the single chamber solid oxide fuel cell and it can provide a basic for the design, scale up of single chamber solid oxide fuel cell system.

1. Introduction

As a clean and efficient energy conversion device, the fuel cell is currently considered as one of the most promising technologies for future energy demand. Solid oxide fuel cells (SOFCs) have several advantages over other types of fuel cells, including flexibility of fuel used and relatively inexpensive materials due to high temperature operation [1]. Solid oxide fuel cell operated in the single-chamber mode, in which the fuel and oxidant are allowed to mix and anode and cathode reactions take place within the same physical chamber, have attracted recent attention. Since no separation between fuel and air is required, single chamber solid oxide fuel cells (SC-SOFCs) greatly simplify the system design and enhances the thermal and mechanical shock resistance [1]. Mathematical models of SOFCs are effective tools in understanding and investigating effects of various design and operation parameters on SOFC performances, as well as helping in SOFC developments. The modeling and simulation results can be used to optimize and control the fuel cell behaviour, increase the efficiency and performance, and design the system [2]. Therefore, a great number of researches had investigated in SOFC modelling and the internal process simulation based on physical principles. These models range from zero-dimensional (0-D) to three-dimensional (3-D) with different features and point to different research objectives. However, there are not so much report on modelling of SC-SOFCs compare to dual chamber SOFCs. The models developed so far are mainly limited to two-dimensional analysis, only few studies developed...
three-dimensional model. Chung and Chung [3] developed a 3D model for a Hibino B-type SC-SOFC fed by hydrogen and solved using FEMLAB. Akhtar et al. [4] model a planar type SC-SOFC fed by hydrogen using 3D analysis.

In this study, we investigate a 3D analysis of a planar type SC-SOFC fed by methane. The model is solved by COMSOL Multiphysics software and compare to the experimental data from our previous study [5].

2. The model

2.1. Experimental set up

The detail of experimental set up could be found in our study [5]. The brief summary of the cell is explained as follows. The anode-supported cell was a porous support of nickel oxide and 10 mol% Gd-doped CeO$_2$ (NiO+GDC). The electrolyte was La$_{0.5}$Dy$_{0.2}$Mo$_2$O$_9$ (LDM). There was a single interlayer of 0.5 wt% Fe$_2$O$_3$-doped Gd$_{0.1}$Ce$_{0.9}$O$_{1.95}$ (Fe-GDC), which functioned as a diffusion barrier to prevent reaction between the LAMOX and the cathode. The cathode layer was La$_{0.6}$Sr$_{0.4}$Co$_{0.8}$Fe$_{0.2}$O$_3$ (LSCF). The configuration of the fuel cell system of Ni+GDC/ LAMOX/Fe-GDC/LSCF was shown in Figure 1. The single cell was suspended on two Au wires for current collecting. The cell was positioned above a coil, which prolongs the heating time for the inflow. Both the cell and the coil were housed in a quartz tube, equipped with a neighbouring thermocouple to monitor the cell temperature. An extra Ni1GDC disk was adhered above the anode to activate the anode on-site. The geometry dimension of the system was summarized in Table 1.

![Figure 1. Configurations of single-chamber solid oxide fuel cells (SOFC) and the anode-supported cell based on LDM electrolyte [5]](image)

| Table 1. Geometry dimensions |
|-----------------------------|
| Dimensions                  | Values (mm) |
| Tube length                 | 45          |
| Tube diameter               | 15          |
| Extra disk, anode           | 13.5        |
| Electrolyte diameter        | 0.55        |
| Extra disk, anode thickness | 9           |
| Cathode diameter            | 0.027       |
| Cathode thickness           | 0.15        |
| Extra disk to anode distance| 0.06        |
| Electrolyte thickness       |             |

2.2. Computational domain

2.2.1. Gas chamber

The gas chamber consists of a cylindrical tube with a planar button anode-supported cell of which the geometry was built as Figure 2.
The applicable equations in this domain are continuity equation, momentum equation, material conservation equation.

2.2.2. Gas diffusion electrodes
The gas diffusion electrodes consist of an anode and a cathode which are porous media. The equations for the domains are continuity equation, momentum equation for transport in porous media, the species conservation equation, and the charge conservation equation.

2.2.3. Electrolyte
The electrolyte is considered to be impermeable to gases. Therefore, both the mass flux and velocity normal to all surfaces of the electrolyte are zero. The other equation is the continuity of ionic current.

3. Results and discussions
The model equations were solved using COMSOL Multiphysics 5.0, a commercial finite element method (FEM) based software package.

The experimental data obtained in our earlier study [5] were used to adjust and validate the model. The cell was operated at the total gas flow rate of 350 sccm (standard cubic centimetre per minute) and the methane over oxygen ratio of 2:1. The temperature of the system is of 700 °C. Some of the parameters of the model obtained from the literature [4], some of the parameters obtained from the fitting procedure. The comparison between the experimental results and the model calculation is shown in Figure 3.

From Figure 3, there is a difference between the experimental results and the estimation from the model. It can be explained that some factors were not fully considered in the model. In our model, the energy conservation was not yet considered. Some of the reactions in the cathode and anode domain might be missing in the model. However, the trend of the calculation results is agreed with the experimental data and it can be used for rough estimation of the performance. The agreement could be improved in the later stage when more factors is added for consideration.
Figure 4 shows the mass fraction of different species along the gas chamber. It can be obtained that the methane is consumed along the chamber and the reactions generate the carbon dioxide and water, mainly by the full combustion.

4. Conclusions
In this study, a three-dimensional numerical model of a single chamber solid oxide fuel cell fed by methane was considered. The results show that the model might be used for roughly estimate the performance of the fuel cell. The results show the potential application of the model for the simulation of the fuel cell system. However, the poor fitting results also suggest that more factors should be taken into account in order to improve the model accuracy. The addition factors could be the heat transfer and heat conservation in the system, the other chemical reaction equations in the anode and cathode.

Acknowledgement
This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 104.03-2013.20.

References
[1] Yano M, Tomita A, Sano M and Hibino T 2007 Recent advances in single-chamber solid oxide fuel cells: A review Solid State Ionics 177 3351-3359.
[2] Kakac S, Pramanjaroenki A and Zhou X Y 2007 A review of numerical modeling of solid oxide fuel cells Int. J. Hydrogen Energy 32 761-786.
[3] Chung C-Y and Chung Y-C 2006 Performance characteristics of micro single-chamber solid oxide fuel cell: Computational analysis J. Power Sources 154 35-41.

[4] Akhtar N, Decent S P and Kendall K 2010 Numerical modelling of methane-powered micro-tubular, single-chamber solid oxide fuel cell J. Power Sources 195 7796-7807.

[5] Lo J-C, Tsai D-S, Chen Y-C, Le M-V, Chung W-H and Liu F-J 2011 La2Mo2O9-Based Electrolyte: Ion Conductivity and Anode-Supported Cell under Single Chamber Conditions J. Am. Ceram. Soc. 94 806-811.