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A comprehensive 3-D modeling of a single planar solid oxide fuel cell

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ABSTRACT

The main motivation of the presented paper is to study the amplitude and location of the maximum temperature (T_{max}) and maximum temperature gradient ($\Delta T/\Delta x_{max}$), respectively, as well as the performance parameters of the modeled, single, planar, anode-supported, solid oxide fuel cell (SOFC) with internal methane steam reforming at different operating conditions (i.e. current density and inlet velocity of fuel gas). The reforming reaction and locally increased current density lead to inhomogeneous heat generation within the SOFC that results in inhomogeneous distribution of temperature. Due to the latter, a comprehensive, three-dimensional, thermo-fluid model of the SOFC has been developed and implemented in software package COMSOL Multiphysics® 4.3. The simulation results show that the amplitude and location of the T_{max} and $\Delta T/\Delta x_{max}$ within the modeled SOFC depend on operating conditions. The data about their values can be efficiently used instead of temperature measurements with expensive embedded thermocouples when a realistic, operating SOFC is controlled. The results also show that the current density and the inlet velocity of fuel gas are the key parameters to improve the fuel utilization and the total conversion efficiency.

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Introduction

Fuel cells (FCs) have become attractive as alternative power sources during the last decades since they convert chemical energy of the fuel directly into electrical energy with high conversion efficiency [1]. Some FCs must be supplied with pure hydrogen as a fuel, e.g. proton exchange membrane (PEM) FCs, which operate at low temperatures ($T < 100$ °C), whereas the others can be supplied with different mixtures of fuels, with e.g. hydrogen, methane, natural gas, and carbon monoxide [2]. One of practically interesting FCs, which can be supplied with hydro-carbon fuels, are solid oxide fuel cells (SOFCs), which operate at high temperatures ($T = 650–1000$ °C) [3]. The SOFC consists of a positive electrode (cathode), solid oxide (electrolyte) and negative electrode (anode) sandwiched between the metal contacts, as can be seen in Fig. 1a. The contacts are commonly made of ferritic (Fe) alloys with chrome (Cr) or nickel (Ni). They serve to conduct electric current from the cathode to the external load and from the load back to the anode, or to interconnect many cells in parallel or/and in series into the stack. Besides this, the contacts form the fuel- and air-flow channel adjacent to the anode and cathode side of the SOFC, respectively. The anode is usually porous nickel/yttria-stabilized zirconia (Ni/YSZ) material, the electrolyte is dense YSZ and the cathode is porous lanthanum manganite ($LaMnO_3$)

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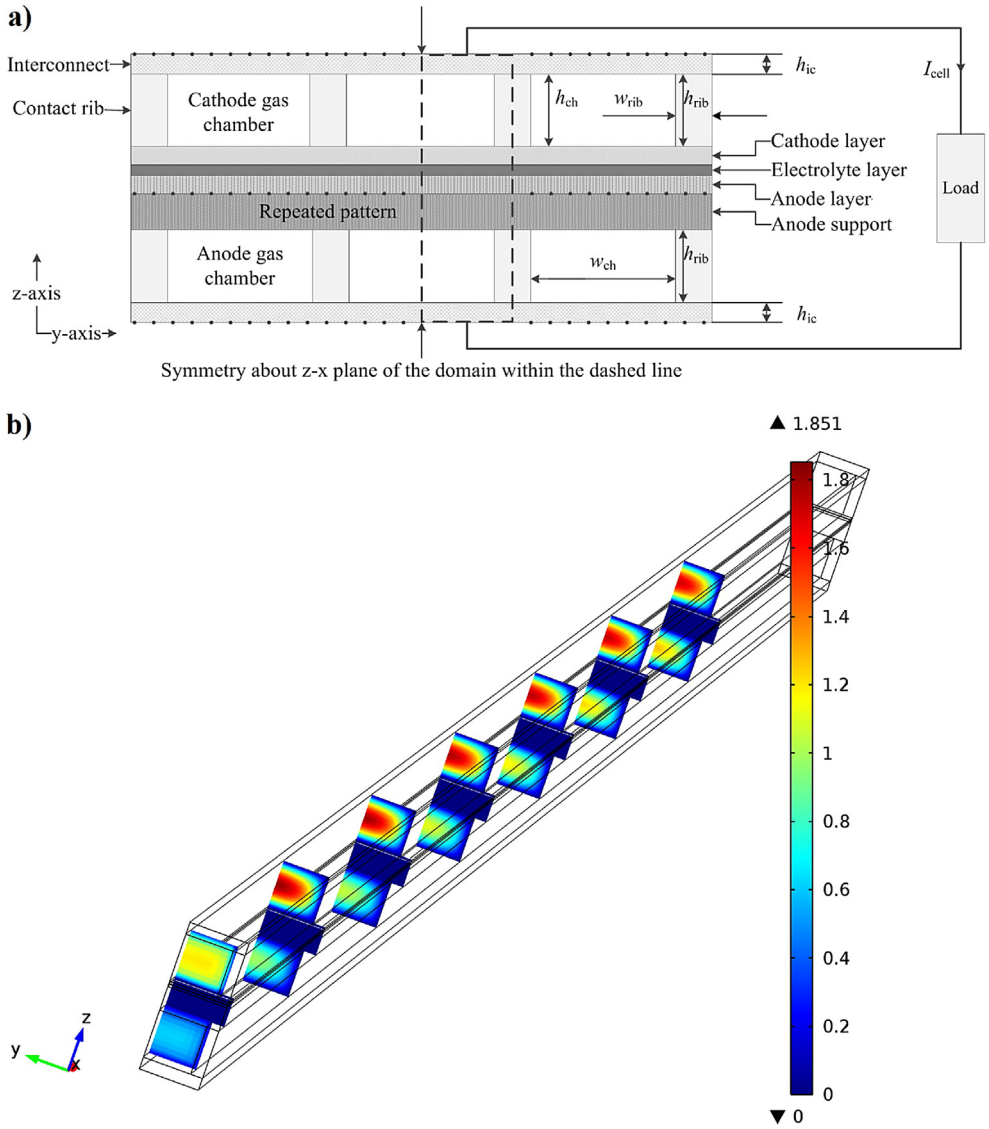

Fig. 1 – a) Cross-section profile of the modeled solid oxide fuel cell (SOFC) with external load, b) Velocity field (in m s^{-1}) of gas species in the modeled SOFC structure.

doped with strontium (LSM) [4]. Under the operation of SOFC (i.e. the FC is supplied with inflow of air and fuel), the following electrochemical reactions occur within triple phase boundaries (TPBs are thin boundaries between the electrode and electrolyte micrograins surrounded with gaseous phases that fill the pores) at the interfaces between the electrolyte and cathode (1 – reduction), and electrolyte and anode (2, 3 – oxidation) catalyst layer:

$$\frac{1}{2}O_2 + 2e^- = O^{2-}, \tag{1}$$

$$H_2 + O^{2-} = H_2O + 2e^-, \tag{2}$$

$$CO + O^{2-} = CO_2 + 2e^-. \tag{3}$$

The oxygen is thus adsorbed within the TPBs at the interface between the electrolyte and porous cathode and the oxygen ions are transferred through the dense electrolyte to the interface between the electrolyte and porous anode, where the oxidation of hydrogen/carbon monoxide occurs within the TPBs. The flow of oxygen ions through the electrolyte represents electric current density that is in the opposite direction since the ions are negatively charged. The flow of electrons is terminated through the load, which is connected to the contacts, and it represents the output current density of the SOFC. The electrons exit the anode side and enter the cathode side of the SOFC through the contacts and load. The output current density is thus directed from cathode to anode side through the electric load since electrons are negatively charged. The physical background behind the operation of a SOFC is far more complex as explained before and cannot be described in all details at this point.

In this paper, the study is based on physical model that consist of coupled partial differential equations when spatial variations of dependent variables are considered. The models are conditioned by the purpose of application. Many different

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