Research Paper

Effect of catalyst layer configuration on single chamber solid oxide fuel cell performance

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HIGHLIGHTS

- Performance analysis of three different SCSOFC catalyst layer configurations is done.
- The ohmic loss plays a key factor in performance enhancement.
- Stacking the perpendicular configuration cell enhances the SCSOFC performance.

ARTICLE INFO

ABSTRACT

The purpose of the current study is to numerically evaluate the effect of coplanar and perpendicular catalyst layer configurations on the performance of a single chamber solid oxide fuel cell (SC-SOFC). Three different catalyst layer configurations, coplanar, single-cell perpendicular and two-cell stack are used. Fuel is a mixture of hydrogen and air (50% hydrogen and 50% air by volume). An in-house computational fluid dynamics code is utilized to solve the nonlinear governing equations of mass, momentum, energy, charge balance and gas-phase species coupled with kinetics equations. Results show that the perpendicular catalyst layer configuration is more suitable for SC-SOFC than the coplanar configuration. This is due to shorter path of the oxygen ion transportation from cathode to anode in perpendicular compared to coplanar configuration. In addition, results indicate that adding another anode and cathode electrode on the other face of the electrolyte and providing a simple two-cell stack improve the cell performance. Finally, in order to present a suitable configuration of a SCSOFC two-cell stack, a parametric study is performed.

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1. Introduction

Fuel cells directly produce electricity from the external supply of fuel and oxidant [1]. Among different types of fuel cells, solid oxide fuel cells (SOFCs) have gained consideration due to their efficiency and fuel flexibility [2–9]. As known, SOFCs operate in the high temperature range, 700 °C–1000 °C, and face several problems such as material degradation and gas leakage. The gas leakage is the major obstacle of SOFCs for commercialization [2,4,5]. An alternative to SOFC and its mentioned problems is the use of SC-SOFCs. In SC-SOFC, a mixture of fuel and oxidant is fed directly into the cell [5].

The goal of much research is to improve the performance of the SC-SOFCS. To date most research is limited to experimental evaluation of the SC-SOFC which only provides information about overall performance of the cell [2,4,7,10–17]. The few existing papers on

SC-SOFC numerical models do not provide detailed information about the electrochemical interactions which is needed to improve the performance of SC-SOFC [3,6].

A study by Chung et al. [3] shows that ohmic loss is the major loss in the SC-SOFCs compared to the other two losses (i.e. concentration and activation losses). Their results also reveal that the ohmic loss diminishes by increasing the electrolyte layer thickness. The same results are presented by Akhtar and his team [12]. They reported that increasing the electrolyte layer thickness extends the cross-sectional area available for ionic current flow in lateral direction. Akhtar also evaluated the effect of the cathode to anode distance on gas species as well as the velocity distribution through electrodes. The right-angular configuration for SC-SOFC was initially introduced by Wang et al. [13]. They used methane–air mixture as fuel for this configuration. Wang reported that the right-angular configuration exhibits much better performance than coplanar configuration. This is due to considerable reduction in the ohmic resistance occurring in right-angular type. They also studied the two-cell right-angular configuration stack performance and found out

that the ohmic resistance is the smallest in this configuration. However, their results are limited to experiments and just give information about the overall performance of the cell.

The main aim of the current study is to look at the effect of different catalyst layer configurations on the cell performance. The goal is to advice an anode and cathode setup that minimizes the overall losses and increases the SC-SOFC performance.

2. Problem definition

Fig. 1 depicts the schematic of the problem. As shown, a mixture of hydrogen and air (50% hydrogen, 50% air by volume) is used to ensure the system safety. The hydrogen is sufficiently diluted with nitrogen to avoid explosion in the system. As shown by Fig. 1 the positive electrode, electrolyte and the negative electrode (PEN) are placed at the middle of the channel. Three different configurations are selected: coplanar configuration (case 1) in which two electrodes are placed on the same side of the electrolyte, perpendicular configuration (case 2) in which electrodes are placed on two mutually perpendicular planes and a two-cell stack in which two single cells are placed on the electrolyte layer to form a simple stack (case 3).

The cell consists of five layers: anode made of nickel (Ni), anode catalyst layer made of nickel–yttria-stabilized zirconia (Ni-YSZ), electrolyte made of yttria-stabilized zirconia (YSZ), cathode catalyst layer made of yttria-stabilized zirconia-lanthanum strontium manganite (YSZ-LSM) and cathode layer made of lanthanum strontium manganite (LSM). Table 1 shows the geometrical parameters.

The fluid is assumed to behave as an ideal gas and the flow is steady, two-dimensional, compressible and laminar. All fluid properties vary with temperature. The electrolyte is fully impermeable and the electrodes are selective which means the following reactions occur in the electrodes:

Anode oxidation of hydrogen:

$$H_2 + O^{-2} \rightarrow H_2O + 2e^- \tag{1}$$

Cathode reduction of oxygen:

$$O_2 + 2e^- \rightarrow O^{-2} \tag{2}$$

Table 1
Geometrical data.

Description	Symbol	Value
Channel width	W_{ch}	150 [mm]
Channel height	H_{ch}	25 [mm]
Anode thickness	t_a	70 [μm]
Anode catalyst layer thickness	t_{ac}	5 [μm]
Electrolyte thickness	t_e	3 [mm]
Cathode thickness	t_c	50 [μm]
Cathode catalyst layer thickness	t_{cc}	5 [μm]
Electrolyte width	W_e	10 [mm]
Electrode width	W_{elec}	2 [mm]
x-Value of electrolyte to anode distance (edge to edge)	d	1.5 [mm]

The ohmic resistance due to electron transport and thermal diffusion is neglected. This is due to the electronic conductivity of the electrodes that is noticeably higher than the ionic conductivity. The inertia term (Stokes–Brinkman's assumption) is also neglected.

2.1. Conservation of mass and momentum

The continuity equation is as follows [14]:

$$\nabla \cdot (\rho \mathbf{u}) = \sum_j R_j \tag{3}$$

in which ρ is density of the mixture and $\mathbf{u}$ is velocity vector. The right hand side of Eq. (3) accounts for mass depletion or creation due to electrochemical reactions (i.e. Eqs (1) and (2)). The mass source term is zero for other layers because electrochemical reactions occur in the catalyst layers.

The momentum equation in the porous electrodes based on Darcy's law is expressed as [14,18]:

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-p\mathbf{I} + \frac{\mu}{\varepsilon} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \frac{2\mu}{3} (\nabla \cdot \mathbf{u})\mathbf{I} \right) + \rho \mathbf{g} - \left(\frac{\mu}{\kappa} \right) \mathbf{u} + \mathbf{F} \tag{4}$$

where μ is the dynamic viscosity of the fluid, and ε and κ are porosity and permeability of porous electrodes respectively and $\mathbf{F}$ is the volume force acting on the fluid. By applying
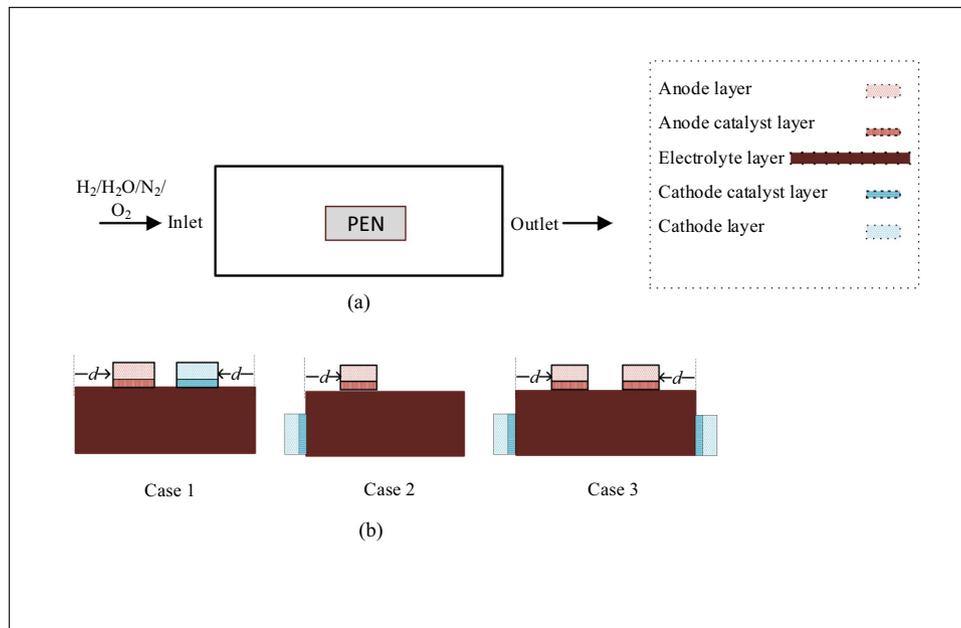

Fig. 1. The schematic of the problem: (a) the whole computational domain with the inlet and the outlet; (b) different catalyst layer configurations considered in modeling.