Micro-Solid Oxide Fuel Cell: A multi-fuel approach for portable applications

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HIGHLIGHTS

- We report the oxygen ion transport properties at the electrode–electrolyte interface (EEI) of the SOFC for the first time.
- This ion transport plays a key role in the overall performance of SOFCs with different fuels.
- The GIIB mechanism is also studied for the first time.
- GIIB is assumed to be the prime reason for low power density and ion conductivity at the EEI when using hydrocarbon fuels.
- Due to its scalability, a fuel cell can serve as a power source for on-chip applications and all portable equipment.

ARTICLE INFO

ABSTRACT

The impact of oxygen ion transport at the electrolyte–electrode interface of a micro-solid oxide fuel cell using different fuels is investigated. Model validation is performed to verify the results versus the reported values. Furthermore, as the hydrogen-to-carbon ratio decreases, the diffusivity of the oxygen ion increases. This increase in diffusivity is observed because the number of hydrogen atoms available as the reacting species increases in fuels with lower hydrogen-to-carbon ratios. The oxygen ion conductivity and output power density decrease as the hydrogen-to-carbon ratio of the fuels decreases. The reason behind this impact is the formation of a gas-induced ion barrier at the electrode–electrolyte interface by the CO_2 molecules formed during the reaction at the interface, thus blocking the flow of oxygen ions. As the oxygen ions become blocked, the output current contribution from the reaction also decreases and thereby affects the overall performance of the micro-solid oxide fuel cell. The experimental verification confirms this because of a significant decrease in the output power density. Furthermore, as per the application in portable devices, the appropriate choice of fuel can be chosen so that the micro-solid oxide fuel cell operates at the maximum power density.

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1. Introduction

An electrolyte sandwiched between two porous electrodes serves as the basic blocks of a fuel cell. Near-zero emission, noise-free operation and ease of scalability make the fuel cell a prime candidate for creating a sustainable economy by providing a local- and nation-wide power system and thus for lowering the greenhouse effect in the environment. Fuel cells have very high efficiencies and can replace the internal combustion engines in the near future. In addition, *due to its scalability, a fuel cell can serve as a power source for on-chip applications and all portable equipment.*

Referable to high efficiency, capability of working with a wide range of fuels, and modular design options like tubular and planar,

solid oxide fuel cells (SOFC) have drawn the engrossment of many researchers. The tubular one has the advantage that sealing is more comfortable whereas, the planar one is superior in terms of efficiency and ease of manufacture and stacking.

Last two decades have seen enormous research publications pertaining to SOFC. Numerical studies focus on modeling the coupled physical and chemical and electrochemical phenomena occurring in the cell/stack, however experimental studies, mostly focus on the evaluation of possible materials and/or fuels. Numerous sophisticated mathematical models are published for the tubular, planar, integrated planar and monolithic designs thus far [1–17]. These models for SOFCs serve as important tools in understanding and examining the effects of various design and operation parameters on SOFC performances as well as in SOFC developments.

A three-dimensional (3D) approach to model the whole cell/stack has been looked upon [8, 18–20]. These focused on the

impact of the configuration and operating conditions on the overall performance of the cell/stack. However, simplification of phenomena occurring within the ensemble of positive electrode–electrolyte–negative electrode (PEN) are attributed.

Two-dimensional (2D) models are popular with tubular solid oxide fuel cells because of their axial symmetry [21–24]. Others have employed a quasi-2D models planar designs [25–26], which address one-dimensional fluid flows in the channels with the transverse gas transport in the porous electrodes by boundary conditions at the channel-electrode interfaces.

In one-dimensional (1D) approaches the PEN structure is seen as a thin layer separating the fuel and the air channel flows [27–28], thus the micro processes occurring within the PEN are not observed.

Few research groups [24, 29–37] have concentrated on the analysis of phenomena taking place locally in the porous electrodes and/or in the electrolyte, these include polarization mechanisms, charge transfers and heterogeneous reactions.

Recknagle [19] demonstrated a 3D planar SOFC stack model for predicting the dispersion of the gas species, the temperature and the current. Star-CD was employed to investigate three configurations of co-, counter- and cross-flows delineating that the co-flow configuration generates the best uniform temperature and therefore the smallest temperature gradients.

Nevertheless, detailed transport processes in the porous electrodes and electrolyte were not simulated numerically as the PEN structure was treated as a single solid layer. Rather, empirical models were used for potential losses, and chemical species variations due to electrochemical processes were instituted into the channel streams as boundary conditions at the PEN-channel interfaces.

Chan and Xia [2] presented a 1D anode model of a micro-SOFC, which consisted of the transport of ion, electron, and gas molecules through the porous anode and the three-phase boundary (TPB) electrochemical reaction of the anode. They concluded that an overall polarization reaches a minimum at a certain particle size. When pure hydrogen is used, very high anode polarization is achieved, and thus the anode thickness and particle size in an anode design are inter-related with each other. For providing sufficient reaction sites, the particle size should be larger and should be a thick anode.

In 2003, Pasaogullari and Wang [8] developed a multi-physics, multi-dimensional model to simulate SOFCs, to predict the polarization curve, species concentrations, and current distributions. They used the commercial CFD program, FLUENT. The model fully combined electrochemical kinetics with the multi-dimensional gas dynamics and multi-component transport of species. It also solved the continuum equations for the conservation of species, mass, momentum, electric charge, and thermal energy along with electrochemical kinetics in the cathode and anode of a planar SOFC. They also mentioned that their model served as a building block for a complete CFD-based model for an internal reforming-anode SOFC.

Abakevičienė et al. [15] used the Comsol Solid Mechanics module to model a 2D geometry of the cross-sectional micro-SOFC structure. They studied the normal stress distribution in the micro-SOFC structure with a sacrificial layer of Si_3N_4 and showed that at high temperatures, the substrate expanded less than the coating, instigating tensile stresses in the substrate area next to the coating and compressive stresses in the coating because the substrate material had a lower thermal expansion coefficient than the layered Pt/YSZ/Pt coating.

Navasa et al. [17] developed a three-dimensional FVM based CFD model for a cathode-supported SOEC. They investigated and analyzed the effect of different operating voltages on cell performance.

Further cross-flow and parallel-flow configurations were compared and differences were identified.

Hussain et al. [38] shows a mathematical model predicting the performance of planar solid oxide fuel cell (SOFC) has been developed. The model developed is fuel flexible, and can be used with not only pure H_2 but also any reformate composition (H_2, H_2O, CO, CO_2 and CH_4) as fuel. The model can forecast the performance of SOFC at various operating and design conditions. The model is validated with the measured data found in the literature and shows excellent agreement between the predicted performance and the experimental results. Additionally, the effect of various operating and design parameters on the performance of SOFC has been examined. It is shown that even at higher current densities, the anode concentration overpotential in an anode-supported SOFC is about four orders of magnitude smaller than the anode ohmic overpotential. Further, it is concluded that the losses resulting from ohmic overpotential needs to be minimized to enhance the cell performance.

Cinti et al. [39] identifies the potential of urea as a fuel for fuel cell power systems was investigated. A system operating with diluted urea was modeled integrating the steam reforming of the solid fuel. Efficiencies up to 55% at 800 °C were reported.

Recently, it was also predicted that the micro-solid oxide fuel cell (μ-SOFC) could be used to power a co-generating gas burner [40], micro-hybrid vehicle [40], electronic devices, including communications in remote locations where gas is easily available [41], and portable electronic devices, such as MP3 players, laptops, and mobile phones [42]. Thus, carrying H_2 seems to be risky, so it will be a good idea to have alternative fuels for powering the μ-SOFC [43].

In this work, we report the oxygen ion transport properties at the electrode–electrolyte interface (EEI) of the SOFC for *the first time because this ion transport plays a key role in the overall performance of SOFCs with different fuels*. We have utilized COMSOL platform to model the impact of hydrogen, methane and propane fuels respectively on the transport properties of oxygen ion at the electrode–electrolyte interface (EEI) in a micro solid oxide fuel cell (μ-SOFC). It has been observed that when a low hydrogen to carbon ratio fuel is used, the diffusivity is seen to increase and the oxygen ion conductivity at the EEI is seen to decrease. The prime reason for the decrease in ion conductivity is due to the formation of Gas Induced ion Barrier (GIIB) at the EEI because of the obstruction created by the CO_2 molecules for the flow of oxygen ions at the EEI. This is experimentally verified by observing a significant drop in the output power density of the μ-SOFC. The key motto of this work is to have an on-chip power source for portable gadgets with fuel flexibility as in the device can be operated with any available fuel without the need of changing the fuel cell itself according to the fuel chosen. One of the application of this is to have an in-vivo power source using body fluids as fuel [44–46] to power various body implants, e.g. flow sensing of cerebrospinal fluid in the implanted shunt tube [47–49].

2. Modeling details

The μ-SOFC is made up of an electrolyte sandwiched between two porous gas diffusion electrodes (GDEs) as shown in Fig. 1. The domains corresponding to the components in this model are the cathode and anode interconnects (ribs), air channel, anode and cathode, electrolyte and fuel channel facilitating the study of the flow, electrochemical and thermal effects [50,51]. The various geometric parameters are tabulated in Table 1.

Nickel–Yttria-stabilized zirconia (Ni–YSZ) cermet is used as electrode, and GDC is used as electrolyte material [52]. The GDC material properties were taken from the experimental work [53].