

# Multi-Fuel Modeling of Oxygen Ion Transport in Solid Oxide Fuel Cell

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*Abstract:* - The multi-fuel modeling of Solid Oxide Fuel Cell for hydrogen and methane has been investigated in this work. The main emphasis in this modeling is given to study the oxygen ion transport through the electrolyte. The temperature dependence study of the oxygen ion conductivity, flux and mobility is explored. It is seen that when methane is used as a fuel, the performance of the fuel cell is enhanced. The reason for this enhancement has been explained with appropriate plots.

*Key-Words:* - **Solid Oxide Fuel Cell, Modeling, Ion Transport, Ion Conductivity, Mobility, Flux, Gadolinium doped Ceria.**

## 1 Introduction

William Grove conducted the first known demonstration of the fuel cell. It operated with separate platinum electrodes in oxygen and hydrogen submerged in a dilute sulfuric acid electrolyte solution, essentially reversing a water electrolysis reaction. High temperature solid oxide fuel cells (SOFC) began with Nernst's discovery of the still-used YSZ solid-state ionic conductor [1]. Fueled by technology advances allowing greatly enhanced performance, continuing environmental concern, and a need to develop future power systems that are independent of petroleum fuel stock [2], interest in all types of fuel cell systems for

stationary, automotive [3], and portable power applications is now very high. In all of these applications, there is a need for reduced system cost, high reliability, and acceptable performance. While the performance of many systems has made the greatest strides, there is still much work to be done.

The fuel cell is a high efficiency energy converting system. For optimal performance and design, accurate system modeling for prediction of performance as a function of the myriad of possible operating conditions and transients is needed, but such modeling requires an understanding of all relevant phenomena. Although the fundamentals of operation are couched in basic electrochemistry,

advances in all areas are made in such a rapid fashion that it is nearly impossible for one researcher to be fully cognizant of all aspects of the state of the art. In order to make strides in the three primary needs of high performance, low cost, and high reliability, one must possess a basic understanding of the principles of electrochemistry, materials and manufacturing, and heat and mass transfer. Because of this highly interdisciplinary nature of fuel cell systems, many successful research programs are built around a team approach involving investigators from complementary disciplines.

The future of power generation will almost certainly include fuel cell systems. The purpose of this article is to provide an overview of the advantages, limitations, and technical challenges of contemporary hydrogen polymer electrolyte membrane, direct methanol, and solid oxide fuel cell technology, with emphasis on critical transport phenomena occurring in these systems.

The basic advantages common to all fuel cell systems are as follows [2]:

- Potential for a high operating efficiency (up to 50-70%), that is not a strong function of system size.
- Zero or near-zero greenhouse emissions, with level of pollution reduction depending on the particular fuel cell system and fuel option.
- No moving parts, except pumps or compressors, thus providing stealthy, vibration-free, and highly reliable operation.
- A highly scalable design.
- Multiple choices of potential fuel feedstock's.
- A nearly instantaneous recharge capability compared to batteries.

Fig. 1 shows a generalized schematic of a fuel cell. Gas-phase fuel and oxidizer streams enter through flow channels, separated by the electrolyte/electrode assembly. Reactants are transported by diffusion and/or convection to the catalyzed electrode surfaces, where electrochemical reactions take place. The electrolyte functions to transport ions created by reaction at one electrode to the other. In SOFC systems, the  $O^{2-}$  ion is transferred. The electrolyte can be a solid ceramic material, such as YSZ,  $CeO_2$  [4]. It is always desirable to reduce electrolyte thickness to reduce internal ohmic losses. However, the electrolyte must also be relatively impermeable to fuel and oxidizer to minimize reactant crossover, stable in oxidizing and reducing environments over time, and maintain structural

integrity at operating conditions. Permeability of the electrolyte to the reactants results in mixed potentials at the electrodes, reducing performance, and possibly degrading the catalyst. The requirements for the electrode include low activation losses, long-term stability, and acceptable ionic/electronic conductivity. In high temperature SOFC systems (with greatly reduced activation polarization) utilize much cheaper catalyst materials such as nickel.

In this work, we studied the modeling of oxygen ion transport through the electrolyte (Gadolinium doped Ceria, GDC) and its variation due to change in fuel from hydrogen to methane in SOFC.

## 2 Modeling details

SOFC is constructed with two porous gas diffusion electrodes (GDEs) [5] with an electrolyte sandwiched in the middle; see Fig. 1. The model comprises of different domains corresponding to the components: the cathode interconnect (rib), air channel, cathode, electrolyte, anode, fuel channel, and anode interconnect (rib) which would facilitate to examine the electrochemical, flow, and thermal effects. The details of these components are tabulated in Table I.

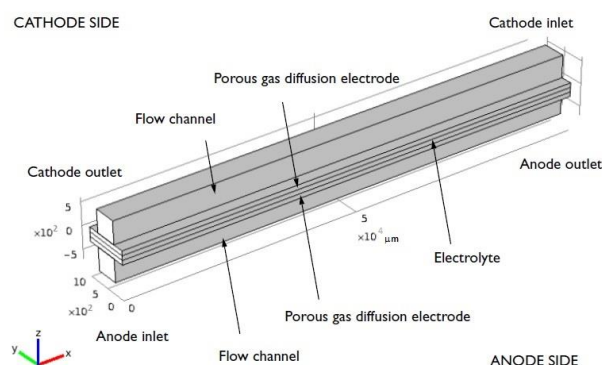


Figure 1. Geometry of the unit cell, with anode at the bottom and cathode at the top.

TABLE I. GEOMETRIC PARAMETERS USED IN THIS MODEL OF SOFC

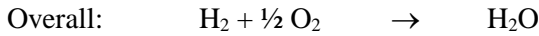
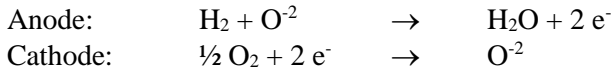
Domains	Value ( $\mu\text{m}$ )
Gas flow channel width	5e+2
Rib width	5e+2
Gas diffusion electrode thickness	1e+2
Electrolyte thickness	1e+2
Gas flow channel height	5e+2
Flow channel length	1e4

The material used for electrodes is Nickel-Yttria-

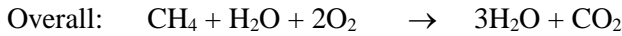
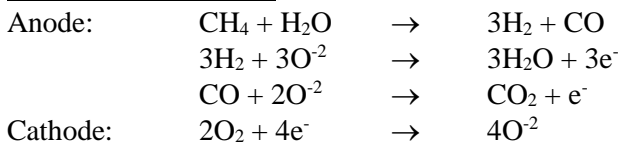
stabilized zirconia (Ni-YSZ) cermet whereas for electrolyte it is GDC. The material properties of GDC were taken from the experimental work [6]

Electrochemical reactions for the anode and cathode for a hydrogen-fed and methane-fed solid oxide fuel cell (SOFC) are-

for hydrogen-fed SOFC,



for methane-fed SOFC,



The model includes the following processes:

- Electronic charge balance (Ohm's law)
- Ionic charge balance (Ohm's law)
- Butler-Volmer charge transfer kinetics
- Flow distribution in gas channels (Navier-Stokes)
- Flow in the porous GDEs (Brinkman equations)
- Mass balances in gas phase in both gas channels and porous electrodes (Maxwell-Stefan Diffusion and Convection)
- Electrostatics for studying the electric field through the electrolyte

At the anode, in case of fuel being hydrogen, a humidified hydrogen gas is supplied as fuel, meaning that the gas consists of two components: hydrogen and water vapor, whereas when fuel is methane, humidified methane gas is supplied as fuel, meaning that the gas consists of two components: methane and water vapor. In the cathode, humidified air is supplied, consisting of three components: oxygen, water vapor, and nitrogen.

The material transport is described by the Maxwell-Stefan's diffusion and convection equations, solved for by using a Transport of Concentrated Species physics interface for each electrode flow compartment.

The boundary conditions at the walls of the gas channel and GDE are zero mass flux (insulating

condition). At the inlet, the composition is specified, while the outlet condition is convective flux. This assumption means that the convective term dominates the transport perpendicular to this boundary.

The governing equations are discretized and solved with the finite element method (FEM) using COMSOL® Multiphysics platform.

### 3 Results and Discussion

Simulations are performed to investigate the oxygen ion transport through the GDC electrolyte in SOFC's at various temperature range and also its dependence with different fuels as hydrogen and methane.

As shown in fig. 1, the ionic conductivity of oxygen ions through the electrolyte increases with temperature which is more prominent in the case of methane as compared to that of hydrogen.

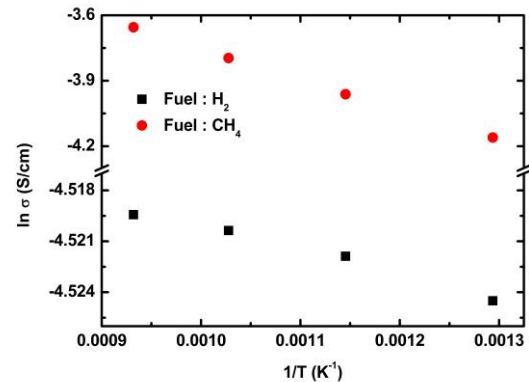


Figure 2. Temperature dependence of ionic conductivity of oxygen ions in GDC electrolyte with different fuels such as hydrogen and methane.

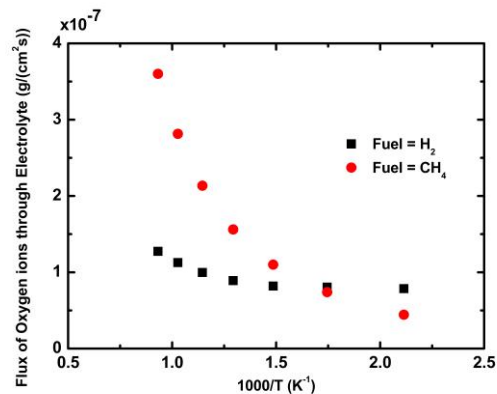


Figure 3. Temperature dependence of flux of oxygen ions in GDC electrolyte with different fuels such as hydrogen and methane.

The temperature and fuel dependence of oxygen ion flux and mobility is also investigated. As seen from fig. 3 the flux of oxygen ions show an exponential increase with rise in temperature. This rise is more significant for methane as fuel since for oxidation of methane four atoms of oxygen are required whereas two atoms are only required for oxidation of hydrogen to form water molecule. It is also observed that at low temperature the flux is lower than that of hydrogen which implies that methane won't react with oxygen at low temperatures and thus the rate of reaction would be low enough in order that the reaction takes place.

Fig. 4 shows the temperature dependence of mobility of oxygen ions hopping from cathode to anode through the electrolyte. The signature behavior of mobility in semiconductors is seen here, i.e. as temperature increases there is an exponential decrease in the mobility.

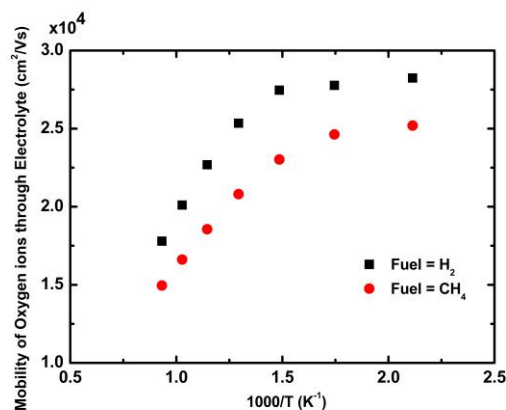


Figure 4. Temperature dependence of mobility of oxygen ions in GDC electrolyte with different fuels such as hydrogen and methane.

The mobility is higher in case of H<sub>2</sub>, because the CO<sub>2</sub> formation as a by – product when CH<sub>4</sub> is being used creates blockages in the electrolyte thus reducing the oxygen ion flow.

## 4 Conclusion

The temperature and different fuel dependence of oxygen ion transport in GDC electrolyte of a SOFC has been modelled and the observed ionic conductivity, flux and mobility variations have been explained.

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