

Numerical modelling of a serpentine channel SOFC for elevated pressure applications

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Abstract

The present study investigates the effect of system pressurization over an anode supported planar SOFC. A three dimensional SOFC model is simulated using a commercial CFD software COMSOL multiphysics. To investigate the cell performance, the model takes into account fluid flow, heat, mass, and charge transport processes, and electrokinetics with suitable boundary conditions. The paper focuses on the impact of pressurization in the range of 1 atm to 4 atm. Alongside the pressure, the temperature is also varied from 1023 K to 1073 K. The study also calculates and analyses all the overpotentials associated with SOFC operation and the resultant heat generation.

Keywords: SOFC, pressurization, Power density, overpotential.

1. Introduction

The advancement of modern society and improvement in quality of life has raised the overall global power consumption to an alarming extent. This, combined with fossil fuel depletion and the dangers of global warming, has brought things to an alarming situation as regards the demand and supply of global energy. Under these circumstances, a power generation device with low emission and high efficiency is highly sought-for [1–3]. Fuel cells are one of the promising alternatives for abating the aforementioned problems. A fuel cell is an electrochemical device that directly converts the chemical energy to electrical energy without any direct combustion of the fuel. In doing so, it achieves higher efficiency by bypassing the conventional Carnot limitations. Solid oxide fuel cells (SOFCs), the subject of this study, have a number of advantages over other fuel cells due to their flexibility with various conventional and renewable fuels, cheap and durable catalysts, and its silent operation. Moreover, the high temperature of SOFCs opens up an avenue to generate power combined with an conventional steam or gas power plant. A hybrid power plant consisting of a SOFC and a gas turbine increases the power generation as well as the electrical efficiency of the hybrid power generation system.

A schematic diagram of a planar SOFC consisting of interconnects (bipolar plates) with serpentine channels is shown in Figure 1 . The pictured unit cell consists of two porous cathode and anode electrodes, a solid dense electrolyte, and a fluid flow channel alongside each electrode. The fluid flow paths depend on the shape of the interconnects and cell performance is known to be highly sensitive to them. The metallic interconnects also collect current from the cell.

Since it is much more economical to compress gases at lower temperatures, in a hybrid SOFC system the fuel and air are compressed before being pre-heated and fed into the SOFC stack and as a result, the SOFC is operated at elevated pressure. This makes an investigation of the electrochemical and mechanical behaviour of SOFCs at elevated pressures a crucial research area. The present work compares the electrochemical and thermal performance of a series of CFD models of pressurised SOFCs with a reference model operating at atmospheric pressure. In addition, the effect of variation of operating temperature on the pressurised SOFCs is also simulated and analysed.

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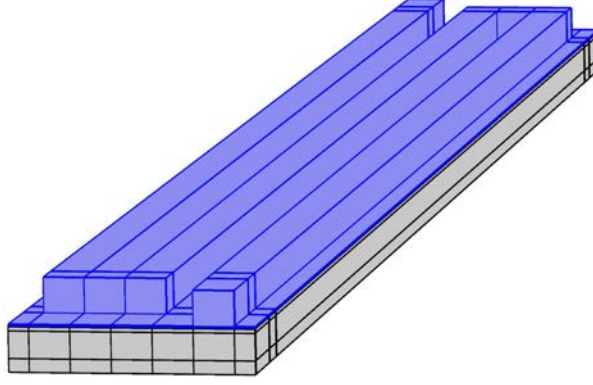


Fig. 1. Schematic Diagram of an SOFC with serpentine channel

2. Methodology

SOFC operation simultaneously involves a diverse blend of physics, including fluid flow, heat transfer, electrochemistry etc; and each of these are defined by their particular equations, and is followed by suitable boundary conditions. In the present paper, all the equations are discretised and solved simultaneously using the commercial CFD software COMSOL Multiphysics. The details of validation with experiments, mesh refinement study is available in our previous communication [4].

2.1. Geometric dimensions

The current planar serpentine SOFC consists of Nickel-doped Ytria Stabilised Zirconia (Ni-YSZ) anode, followed by electrolyte of 8 mol% Ytria Stabilised Zirconia (8-YSZ) and Strontium-doped Lanthanum Manganite cathode.

Table 1. Modelling Parameters

Parameter(Unit)	Symbol	Value/Expression	Source
Anode Thickness (μm)	H_{anode}	150	
Electrolyte Thickness (μm)	$H_{electrolyte}$	30	
Cathode Thickness (μm)	$H_{cathode}$	50	
Anode Flow Channel Height (mm)	H_{aChan}	1	
Cathode Flow Channel Height (mm)	H_{cChan}	1.3	
Interconnect Thickness (mm)	H_{int}	$1.5 \times H_{electrode}$	
Specific Surface Area (m^{-1})	S_g	$1.2\text{E}+5$	[5]
Fuel/Air Inlet Temperature (K)	T_{in}	1073	
Ambient Temperature (K)	T_{amb}	1073	
Ambient Pressure (Pa)	P_{atm}	101325	
Length of the geometry(m)	L	0.09	

2.2. Governing equations and boundary conditions

In the present model, the weakly compressible Navier-Stokes equation is used to compute fluid flow variables in the cathode and anode channels, while the Brinkman equation is used to study flow through the porous medium. Both equations are also coupled with the equation of continuity. These are done using the porous media and subsurface flow module in COMSOL Multiphysics. Mass transport is governed by bulk motion of fluid in the channels as well as by diffusion in the porous electrodes. The Maxwell-Stefan diffusion model is implemented to study mass transport properties using the Transport of Concentrated Species module of COMSOL. The energy equation is used to describe and analyse the heat transfer as well as temperature profile of the present model using the Heat Transfer module. The energy equation, coupled with electrochemical heat generation, assuming the local temperature equilibrium, is solved using the heat transfer module. The potentials at each electrode and the electrolyte are described by electrochemical reaction kinetics using the Secondary Current Distribution module of

COMSOL. The local current densities at each electrode is predicted by concentration dependent Butler-Volmer Equation. Electrochemical mass and heat generation is coupled to the dynamics of transport phenomena and fluid flow using the inbuilt “Reacting flow” Multiphysics module in COMSOL.

The equilibrium voltage of the cell is expressed using Nernst Equation:

$$E_{eq} = E_0 - \frac{RT}{2F} \ln \left(\frac{x_{H_2O}}{x_{H_2} \sqrt{x_{O_2}}} \right) + \frac{RT}{4F} \ln (p) \quad (1)$$

Where, E_0 is the standard cell potential and x is weight fraction of the particular components and p is the total pressure.

Further to that, considering the activation, ohmic, and concentration overpotentials encountered during cell operation, the actual cell voltage can be expressed as:

$$V_{cell} = E_{eq,c} - E_{eq,a} - \eta \quad (2)$$

where η is the total overpotential of the cell, $E_{eq,c}$ is the equilibrium voltage at the cathode side (1.23 V as calculated from Equation 1) and $E_{eq,a}$ is the equilibrium voltage at the anode side (defined as the electric ground).

The volumetric flow rate and the weight fractions of the species are taken as the inlet boundary conditions for fluid flow and mass transfer respectively. At the anode side, 3% wet Hydrogen is considered, while pure air is considered as oxidant in the cathode side. The gas inlet temperature of both the oxidants and fuel is controlled at 1073 K and set as inlet boundary condition for the Heat Transfer Module of the COMSOL Multiphysics modelling environment. For the electrochemistry, the electrode interconnect surface of cathode is considered at the cell operating voltage and the electrode interconnect surface of anode is at ground (0 V). Periodic boundary conditions are applied at all suitable outer boundaries parallel to the flow of the fluid. The model is uniformly meshed using $\sim 10^6$ cuboidal elements customized to be finer near the reacting interfaces. A direct solver, PARDISO, is employed by setting a relative tolerance of 10^{-5} to solve the equations with suitable boundary conditions.

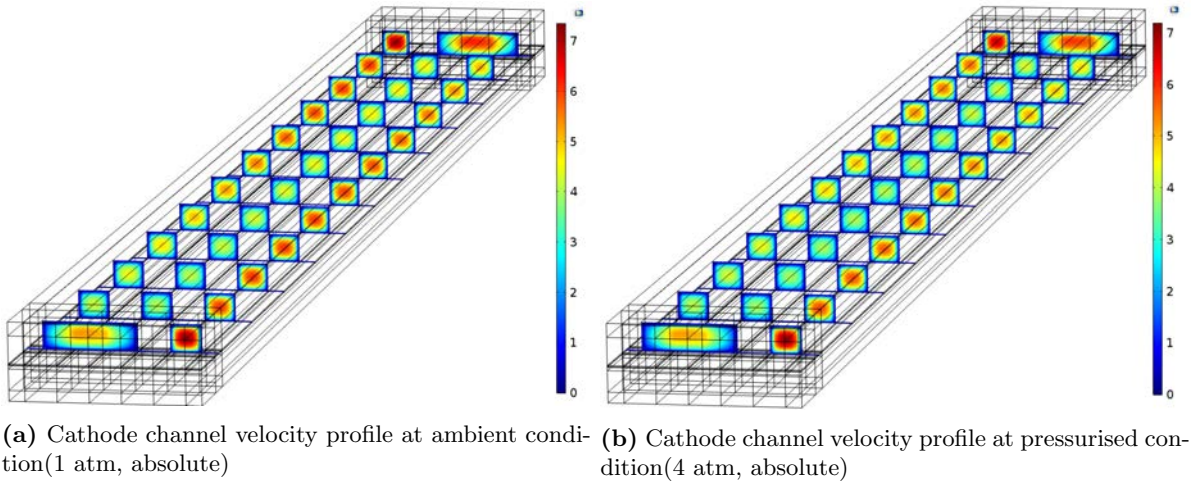


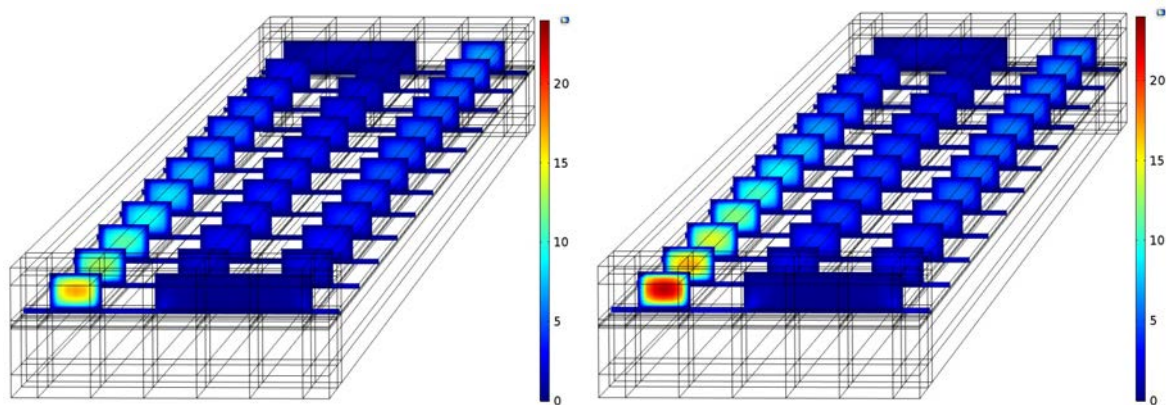
Fig. 2. Velocity profile in cathode channel

3. Results

The electrochemical reaction as well as transportation of gas species dominantly control the electrochemical performance of an SOFC and pressure has a significant effect on both the phenomena. So, it is impossible to deny the effect of system pressurization over the electrochemical performance of SOFC.

Figure 2 shows the cathodic velocity profile of an SOFC working at ambient condition and at elevated pressure of 4 atm. For the sake of representation of the velocity profiles, the analogous domain is sliced into number of slices along the perpendicular plane of the flow direction. Due to no-slip condition, the fluid adjacent to the interconnect wall is always at rest. It is seen that the air velocity at the first segment decreases along the flow channel due to utilization of oxygen. The decrement continues in the second segment and as it proceeds towards the inlet direction again the velocity is raised. With comparison with the pressurized condition, cathode velocity at ambient pressure condition is more due to lack of diffusion.

Figure 3 compares the velocity profile of the anode side and depicts an interestingly reverse behaviour of the cathode side under pressurization condition. The inlet velocity is much higher at elevated pressure with comparison to the SOFC with ambient condition.



(a) Anode channel velocity profile at ambient condition(1 atm, absolute) (b) Anode channel velocity profile at pressurised condition(4 atm, absolute)

Fig. 3. Velocity profile in anode channel

Figure 4 depicts the thermal effect of the current SOFC model at elevated pressure (4 atm absolute pressure). For the inlet fluid temperature of 1073 K, the temperature of the cell is found varying in the range of 1073 K to 1540 K at pressurised condition operating at 0.73 V as shown in Figure 4. The temperature rises along the flow due to exothermic electrochemical reaction. The maximum temperature of the cell is near the fuel inlet; which depicts the electrochemical reaction happens closer to the fuel inlet.

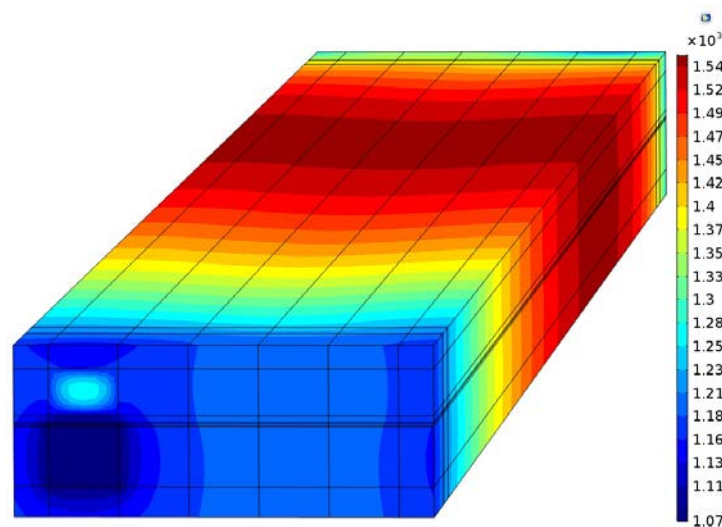


Fig. 4. Temperature profile of SOFC model

Figure 5 depicts the hydrogen distribution along the serpentine flow channel at ambient pressure condition as well as at pressurised condition. It is essential to describe the distribution of hydrogen to analyse the electrochemical reaction characterisation as well as to predict the current distribution of the model. It shows that at elevated pressure, hydrogen concentration is more uniformly distributed; that also helps to predict the uniform current generation at elevated pressure. Non uniformity of current density in plate is one of the major cause of cell depletion; which can be avoided by pressurizing the system.

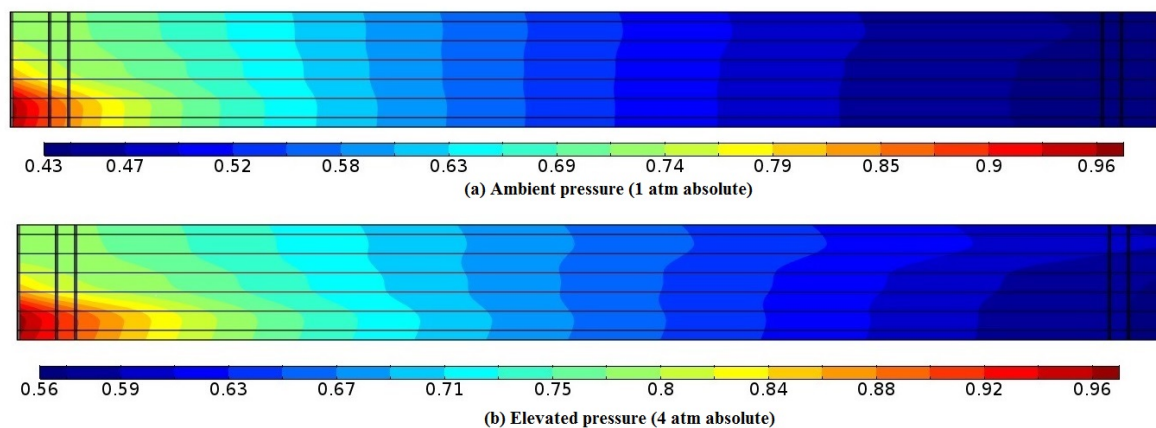
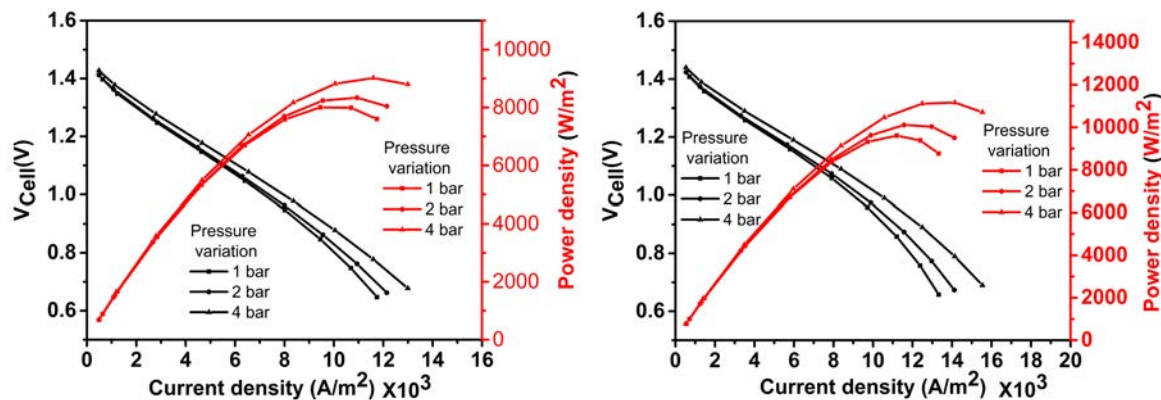


Fig. 5. H₂ concentration along the flow channel

The electrochemical characteristics of the present model with various pressurised conditions at different temperature is shown in Figure 6. Figure 6a depicts the VI characteristics at different pressures when both the fluids inlet temperature is at 1023 K; whereas, Figure 6b shows alike for inlet temperature with 1073 K. Both the plots illustrate that electrochemical performance of cell is increased as the system is being pressurised. The variation in the power output is less at the lower current densities. Comparing both the polarisation plots, the effect of temperature on the performance of pressurised SOFC can be evaluated. The plots depict that the increment in cell performance due to pressurisation of SOFC is more noticeable as the temperature of the inlet flow approaches towards a higher one.



(a) Variation of VI characteristics with pressure at 1023 K (b) Variation of VI characteristics with pressure at 1073 K

Fig. 6. Variation of VI characteristics with pressure

To get a better assessment of the effect of system pressurisation, the total overpotential is calculated with different pressure. Activation, concentration and ohmic polarisation of both the electrodes and the ohmic polarisation of electrolyte are considered into account in the present simulation. The system

pressurisation directly affects the mass transport as well as fluid flow of an SOFC. When the system is pressurised, the diffusional constraints are reduced, as a result the concentration overpotential is reduced. Figure 7 depicts the total concentration overpotential of the cell varied with pressure keeping the cell temperature constant at 1073 K.

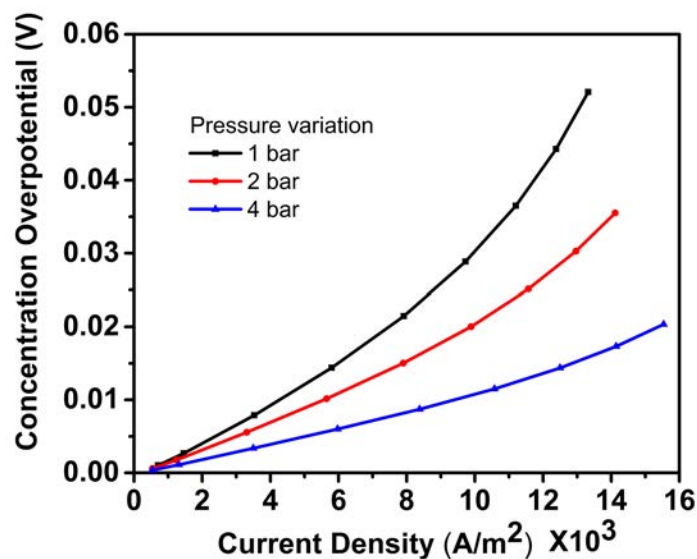


Fig. 7. Variation of total concentration overpotential with pressure

4. Conclusion

In the current study, the influence on an anode supported SOFC performance is analysed numerically. A single serpentine channel SOFC performance is investigated in the (absolute) pressure range of 1 bar (atmosphere) to 4 bar. The Flowing fluid inlet temperature is varied at 1023 K and at 1073 K. It is found that both the flow characteristics as well as electrochemical characteristics are widely affected by the system pressurisation. Pressurisation has the potential to raise the power output of the SOFC model and can reduce the non-uniformity in the current generation along the plate. The overpotential of the cell is also reduced by pressurizing an SOFC. Further, the study also reveals that the effect of pressurization is also increased as the cell temperature is raised.

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