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A PARAMETRIC STUDY OF HIGH TEMPERATURE SOLID OXIDE FUEL CELLS TO OPTIMIZE THE PERFORMANCE

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Abstract: Fuel Cells seem to be a potential solution of our future energy sources. Three dimensional, planar configuration of single solid oxide fuel cell has been modeled in this paper using COMSOL Multiphysics 5.5.0.292 software. The performance of the cell under various operating conditions is studied. The flow of gases is considered to be governed by the Brinkman Equations which represent the combined effect of the Navier Stokes equations and Darcy's Law. From the simulation, the polarization and power characteristics of the fuel cell have been plotted and studied to have optimum output from the fuel cell. The temperature variations, pressure variations, electrolyte conductivity variations, effect of inert gas on the performance and the variation of the exchange current density have been elaboratively studied and the characteristics curves are plotted from the simulation results. The operating conditions were set to approach the real world situation of the various applications of the Solid Oxide Fuel cell. The simulation results help to identify the critical parameters for the optimization of the Solid Oxide Fuel Cell.

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1. INTRODUCTION

A Fuel Cell converts the energy released in a chemical reaction directly to the electrical energy without converting to heat energy [1]. A variety of fuel cells are being studied by the scientific community to have their usage in various fields. A solid oxide fuel cell is a very versatile fuel cell as it employs the electrolyte in a solid state [2, 3]. This makes a solid oxide fuel cell an easy to handle, more durable and highly reliable fuel cell [4]. Moreover they are immune to carbon monoxide poisoning; rather it acts as a fuel [5]. These advantages make the solid oxide fuel cells (SOFCs) to be used as a possible replacement of traditional batteries in most of their applications [6]. The input fuels for the fuel cell are hydrogen and oxygen; however the hydrocarbons are generally used in the fuel cell [7]. In this model, we have used humidified hydrogen as the fuel. Humidified air supplies the required oxygen to the fuel cell. The two react and lead to the generation of energy along with water as the product. Thus a fuel cell is a source of clean and green energy, as product obtained is environment friendly [8]. The typical operating temperature of a solid oxide fuel cell varies from 600°C to 1000°C and thus it is possible to feed the hydrocarbon fuel into the fuel cell where it is converted to hydrogen. Hence the practical difficulties faced in feeding hydrogen directly to a fuel cell are removed in solid oxide fuel cell (SOFC) [9, 10].

Several attempts for the modeling of a fuel cell have already been made. A planar SOFC system was modeled and simulated by Amiri et al. [11] using Aspen plus software. They simulated the working of SOFC using three dimensional stack module. They performed the parametric study of the spatially distributed variables on the performance of SOFC. Zeng et al. [12] developed a three dimensional model of SOFC with optimized interconnect design. Kupecki et al. [13] modeled a planar anode supported solid oxide fuel cell with hydrogen sulphide as the fuel,

operated in direct internal reforming mode. Tikiz et al. [14] developed a computational fluid dynamics (CFD) model and experimentally validated the cell performance in three dimensional planar SOFC [14]. Pirkandi et al. [15] analyzed the performance of a hybrid system of steam turbine, gas turbine and SOFC using EES software. In this model, they studied the energy output of the triple hybrid system and showed that the net power output of such a system is 200% higher than a simple gas turbine system.

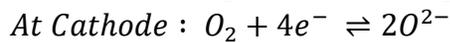
This paper attempts to study the behaviour of a solid oxide fuel cell under various operating conditions. The polarization curve and the output power curves are plotted by varying the conditions of the fuel cell.

2. SOFC OPERATION

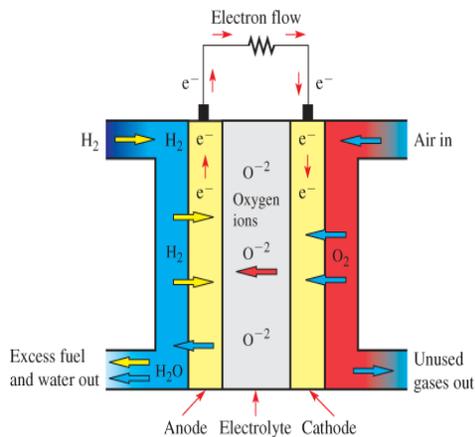
Just like a typical electrochemical cell, a SOFC consists of three basic sections viz. Anode, Cathode and an Electrolyte. The anode material should have significantly high electronic conductivity, should be porous to allow the transport of fuel through itself, and must be thermally and chemically stable [16]. Fergus [17, 18] studied different properties of the materials for their use in SOFC. The commonly used material for anode of a solid oxide fuel cell is Strontium doped Lanthanum Magnetite. Isotomin and Antipov [19] studied the use of the metal oxides as cathode materials in SOFC. For the cathode, the material should be conducting, porous to the flow of the oxidant (oxygen) and should be thermally and chemically stable. Nickel oxide based cermets are the commonly used materials for the cathode of a solid oxide fuel cell. The electrolyte used in SOFC is responsible for carrying the oxide ions from cathode to anode. The material of electrolyte should be porous to flow of oxide ions and should have low thermal conductivity. It must be chemically and thermally stable to work under the high temperature of the SOFC. Yttrium Stabilized Zirconia (YSZ) is the most commonly used electrolyte. The solid electrolyte makes SOFC an easy to handle and relatively more versatile device [20, 21]

A Solid oxide fuel cell has a fuel channel running along the anode. SOFCs can use a variety of fuels like methane, pure hydrogen, Butane etc. The higher operating temperatures of the fuel cell

can be used to convert the hydrocarbon to hydrogen inside the fuel cell itself. In this model we have considered the fuel to be pure hydrogen gas. Similarly, an oxidant is passed through the air channel running along the cathode. In this model we have considered air as the oxidant. The oxygen from air reacts with the metal cathode leading to the formation of oxide ions (O^{2-}). These oxide ions so created at the metal cathode travel through the electrolyte towards the anode [22]. At the anode they combine with the hydrogen (from the fuel) resulting in formation of water. This process liberates two electrons (per oxide ion) which flow from the outer circuit towards the cathode. The flow of these electrons in the outer circuit constitutes the current [23]. The basic reactions taking place at the anode and cathode are written as.



The action of a fuel cell can be shown diagrammatically [24] as below.



OPERATION OF SOFC

Hence, in a fuel cell the energy released in chemical reaction is directly converted to the electrical energy.

3. MODEL DESCRIPTION

Modeling of SOFC involves using the equations of momentum, charge balances, flow of fluid in porous media and charge transfer kinetics. The various equations used to govern the different phenomenas in this model include

1. The electronic charge balance is considered using Ohm's law.
2. The ionic charge balance is considered using Ohm's law.
3. Charge transfer kinetics are studied using Butler Volmer equations.
4. Flow distribution in porous media is studied by implying Brinkman Equations.
5. Gaseous flow in the gas channels viz. the fuel channel and air channel is studied by using Navier Stokes equations.
6. Mass balances of the gases in the gas channels and the porous electrode are studied by Maxwell Stefan distribution and convection is considered.

In this model, we have attempted to model a single SOFC in planar configuration. The modeling has been performed on COMSOL Multiphysics software (version 5.5.0.292). We considered the anode to be made up of Nickel Oxide while the cathode to be made up of Lanthanum Strontium Cobalt ferrite. Yttrium Stabilised Zirconia is the electrolyte considered. The radial flow, both for fuel and the oxidant, is considered at the various operating conditions. The fuel is considered to be a mixture of water vapours and hydrogen i.e. humidified hydrogen is considered as the fuel. The oxidant is considered to be the mixture of oxygen, nitrogen and water vapours i.e. humidified air is taken as the oxidant. We have considered the humidified hydrogen and oxygen as the fuel and oxidant because the presence of water vapours eases the diffusion of the oxidant and the fuel through the porous electrode thus allowing the chemical reaction. All the external boundaries are considered perfectly insulating i.e. zero mass flux condition is implied, to take into account the ionic charge balance. We considered that the Butler Volmer charge transfer kinetics as the governing equations of the charge transfer current density in the SOFC [25]. At the anode, hydrogen combines with the oxygen to form water. Considering that the rate determining step is the step at which first electrons are transferred, the charge transfer kinetic

equation can be written as

$$i_{ct,a} = i_{a,0} \left(\frac{c_{H_2}}{c_{H_2,ref}} \exp\left(\frac{0.5F}{RT} \eta\right) - \frac{c_{H_2O}}{c_{H_2O,ref}} \exp\left(\frac{-1.5F}{RT} \eta\right) \right)$$

Here $i_{a,0}$ is the anode exchange current density, c_{H_2} is the concentration of hydrogen, $c_{H_2,ref}$ is the reference concentration of hydrogen, c_{H_2O} is the concentration of water vapours, $c_{H_2O,ref}$ is the reference concentration of water vapours, R is universal gas constant, T is the absolute temperature, η is the overvoltage and F is the Faraday's constant.

Similarly, the charge transfer kinetic equation at the cathode can be written as

$$i_{ct,c} = i_{c,0} \left(\exp\left(\frac{3.5F}{RT} \eta\right) - n_{O_2} \frac{c_t}{c_{O_2,ref}} \exp\left(\frac{-0.5F}{RT} \eta\right) \right)$$

Here $i_{c,0}$ is the cathode exchange current density, c_t is the total concentration of the species and n_{O_2} is molar fraction of oxygen. All the terms have been considered in SI units.

The overvoltage η is defined as:

$$\eta = V - V_{equil.}$$

Here $V_{equil.}$ is the equilibrium potential difference and V is the electrode potential (in volt).

We have considered the reference potential at the inlet boundary of anode to be zero and at the inlet boundary of cathode to be equal to cell voltage, V_{cell} . The cell voltage is given by

$$V_{cell} = (V_{equil.})_{cathode} - (V_{equil.})_{anode} - V_{pol}$$

V_{pol} is the polarization. The polarization represents the voltage loss due to irreversible phenomenas in the fuel cells. Three major voltage losses occur in a fuel cell i.e. polarization is of three types viz. Ohmic polarization, Activation polarization and Concentration polarization. Ohmic polarization is due to the resistance offered by the various components of the fuel cell. Activation polarization takes into account the voltage loss due to the resistance in the reactions taking place at the surface of electrodes. The concentration polarization represents the voltage loss due to change in concentration of the fuel and oxidant along the length of the fuel cell. In this model we have assumed $(V_{equil.})_{cathode} = 1 V$, $(V_{equil.})_{anode} = 0$. We used the range of polarization i.e. V_{pol} from 0.05 V to 0.80 V so that the cell voltage varies between 0.95 V to 0.20 V. The gaseous flow in the channels is considered to be governed by Navier Stokes

Equation as specified below [26, 27].

$$\rho \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right) = -\nabla p + \nabla (\mu (\nabla u) + (\nabla u)^T) - \frac{2}{3} \mu (\nabla u) I + F$$

Here u represents velocity of the fluid, p is the pressure of fluid, ρ is the density of fluid and μ is the viscosity of fluid. This equation considers four basic parametric forces on the fluid viz. inertial forces of the system $\rho \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right)$, Force exerted by fluid pressure (∇p), viscous forces $\nabla (\mu (\nabla u) + (\nabla u)^T) - \frac{2}{3} \mu (\nabla u) I$ alongwith the external forces applied, F . To drive the gas in the channel, we have set higher pressures at the inlets. We have set a pressure of 6 Pa at the cathode and 2 Pa at anode.

The flow of gases in the gas diffusion electrodes is considered to be governed by Brinkman Equations. The Brinkman Equations represent the combined effect of Darcy's Law and Navier Stokes Equations [28]. The equation used is

$$\nabla p = -\frac{\mu}{k} v + \mu_e \nabla^2(v)$$

Here, μ is the viscosity of the fluid, v is the velocity and μ_e is the effective viscosity parameter.

The material flow in the channels is considered to be governed by the Maxwell Stefan Diffusion and convection in each electrode compartment. At the walls of the channels and the gas diffusion electrodes, we have considered the condition of zero mass flux. At the outlet, we have considered the flow to be governed by convection only.

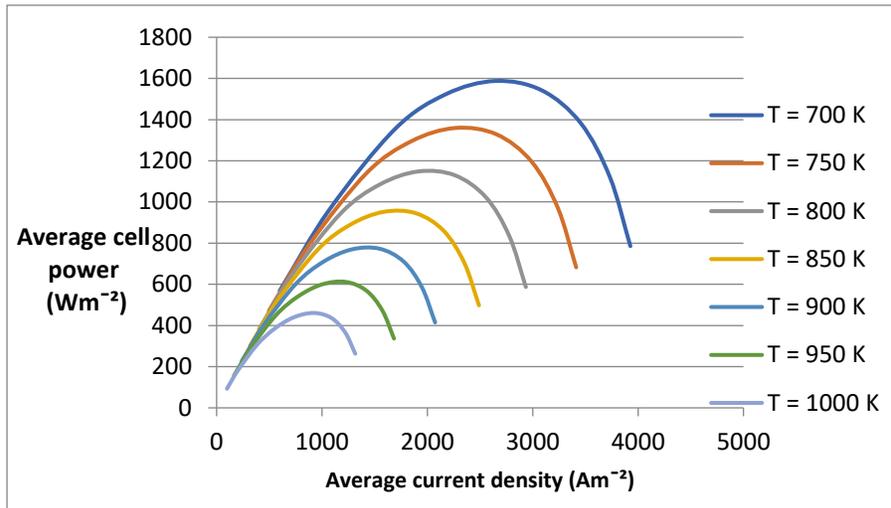
4. RESULTS AND DISCUSSION

A single high temperature SOFC in a planar configuration was modeled and simulated for various parameters and the variation of the Cell voltage and the output power was studied at several operating conditions.

(i) Effect of Variation of Temperature

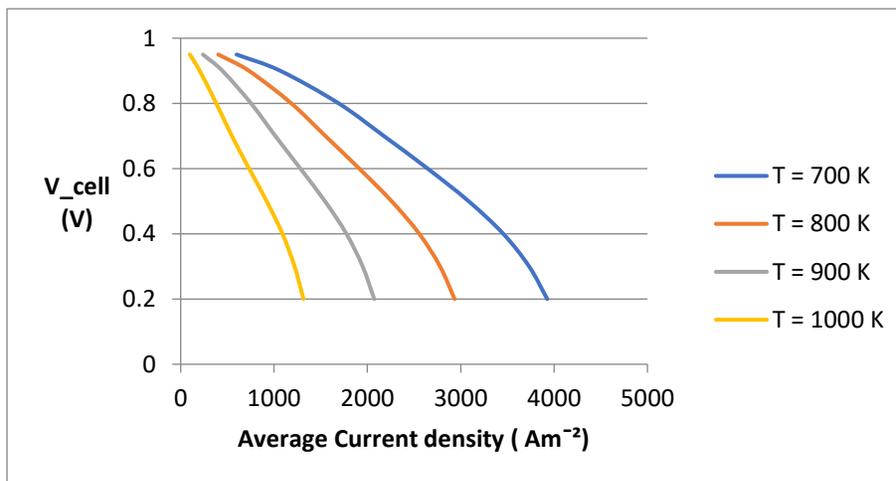
The effect of variation of temperature on the output characteristics of the SOFC was studied. The effect of change of viscosity of the air was also considered during the variation of operating

temperature on the performance of SOFC.



From the graph it is clear that as the operating temperature of the SOFC is increased, the Maximum power output decreases.

The polarization curve variation was also studied at these temperatures. The graphs obtained at the several operating temperatures were as shown.



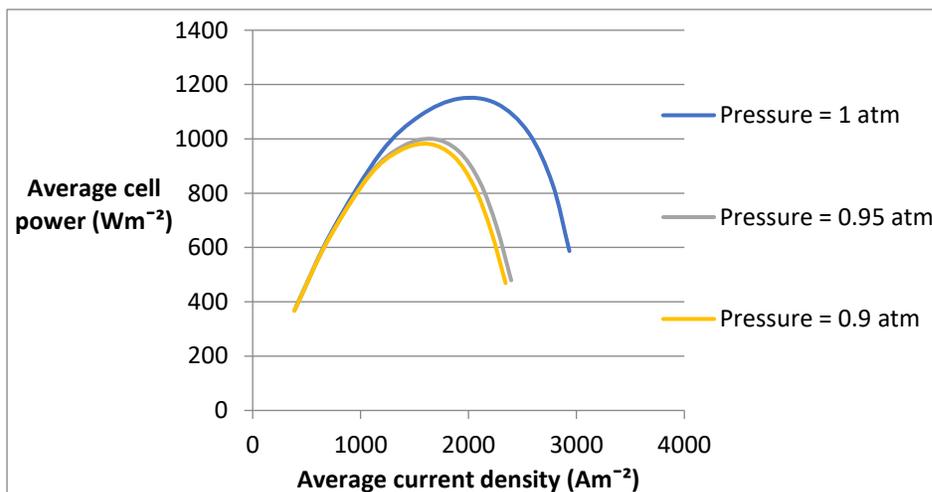
As is evident from the graph, the cell voltage decreases as the temperature of the SOFC is increased

(ii) Effect of variation of pressure

The SOFC was simulated for pressure variations keeping the operating temperature constant (at 800°C, in this case). The variation of the average output power with the average cell current

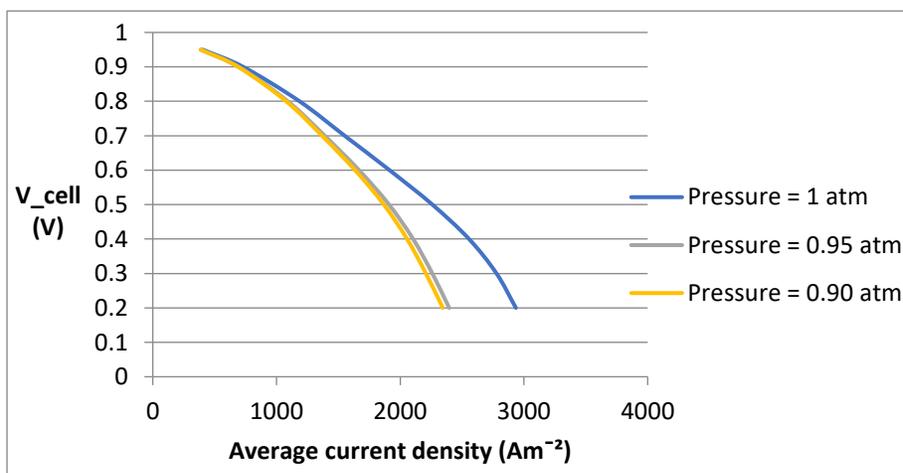
HIGH TEMPERATURE SOFC TO OPTIMIZE THE PERFORMANCE

density is studied at various external pressures.



It is clear from the graph that changing the external pressure from 1 atm to 0.95 atm, changed the power output significantly and further reduction of pressure did not change the output significantly.

Similarly, the polarization curve was obtained at these pressures. The following graphs show the variation of the polarization curves obtained by changing the external pressures.

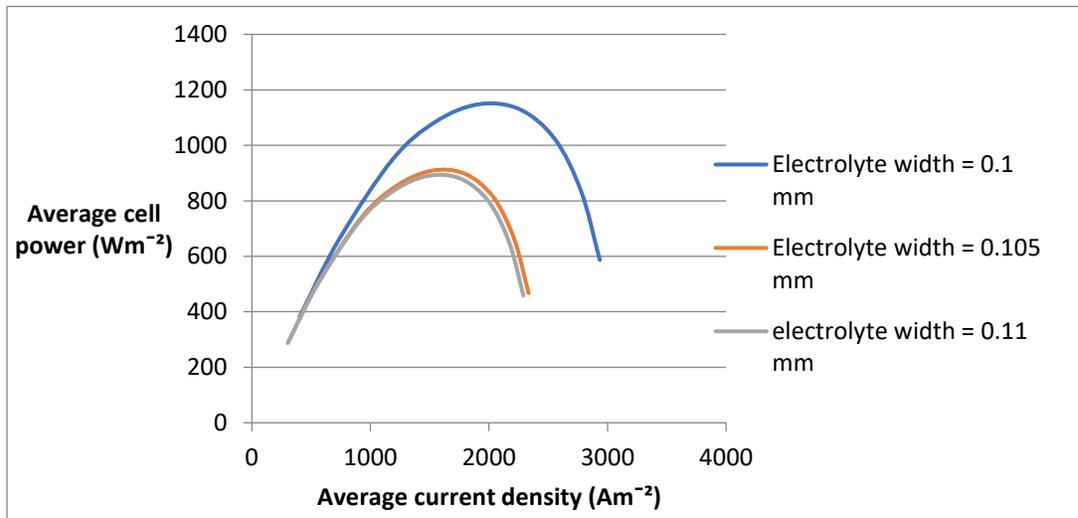


The results obtained are quite show a similar trend that the variation of pressure from 1 atmosphere to 0.95 atmosphere changed the polarization curve significantly, but further reduction

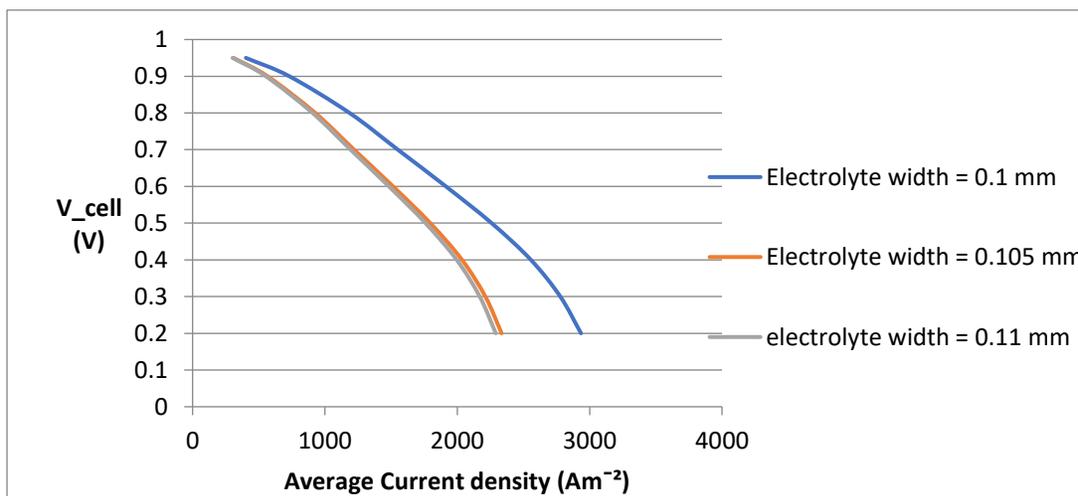
of pressure didn't show significant changes in cell voltage.

(iii) Effect of variation in width of electrolyte

In the model, the electrolyte width was assumed initially to be 1×10^{-4} m. The model was simulated for the variation in the width of the electrolyte and it was found that the slight variations in the width of the electrolyte changed the output considerably. The change goes on decreasing as we go on increasing the width to greater extents.

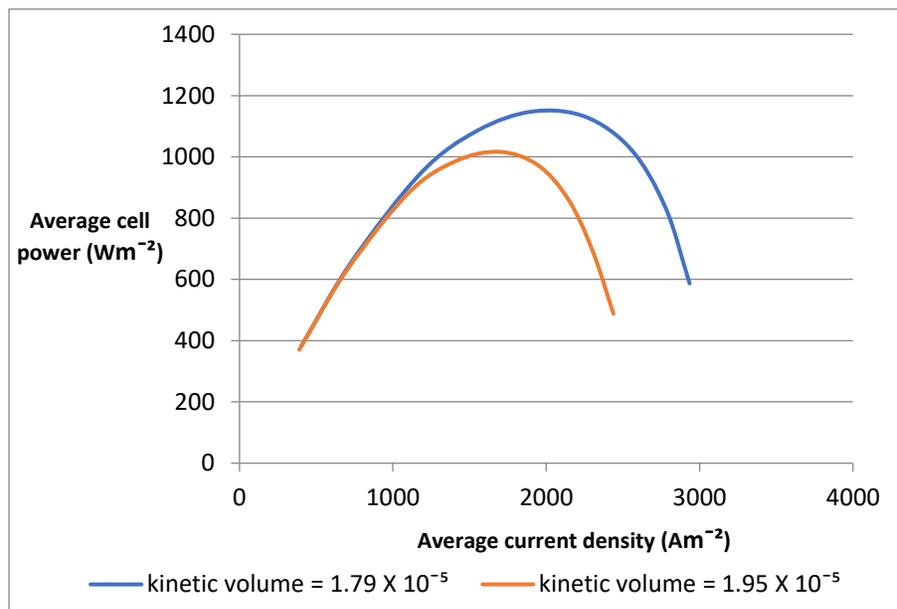


Similar trends were observed in the polarization curve when plotted for these widths of the electrolyte.

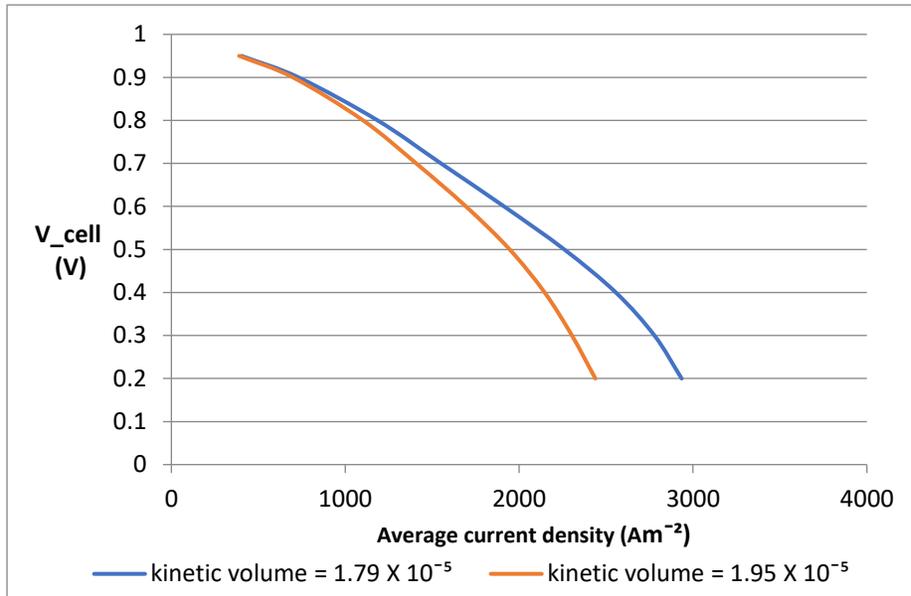


(iv) Effect of inert gas

The oxidant added is humidified air which consists primarily of nitrogen and oxygen. The nitrogen gas does not react with any component of the SOFC and hence is an inert gas. The effect of variation in the kinetic volume on the performance of SOFC was also simulated by plotting both polarization and power characteristics, keeping temperature to be constant at 800°C. It was found that as the kinetic volume of the inert gas increases the maximum power output decreases. This result is in accordance with the fact that as the kinetic volume of the inert gas will increase, the effective oxidant concentration will decrease leading to reduction in the power output.



Similarly, the polarization curve was also plotted for the variation in the kinetic volume of the inert gas at 800°C. The polarization characteristics also show that the output cell voltage decreases as the kinetic volume of inert gas increases.

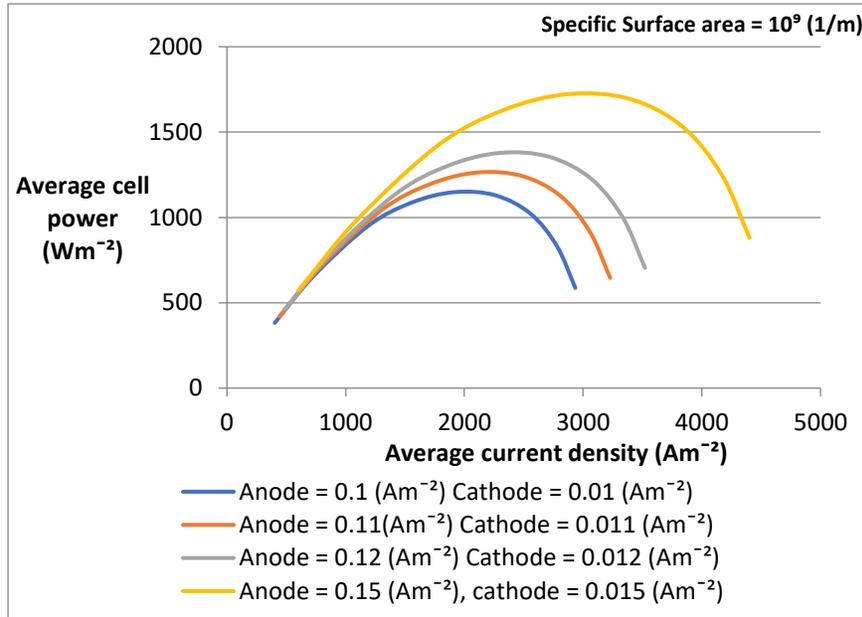


(v) Effect of variation of Exchange Current Density

The exchange current density at anode and cathode play a very significant role in deciding the output of a SOFC by altering the charge transfer kinetics of the reactions occurring in the fuel cell. The fuel cell was simulated for various values of the cathodic and anodic exchange current densities at constant operating temperature of 800°C . Both the power characteristics and the polarization characteristics of the cell were plotted.

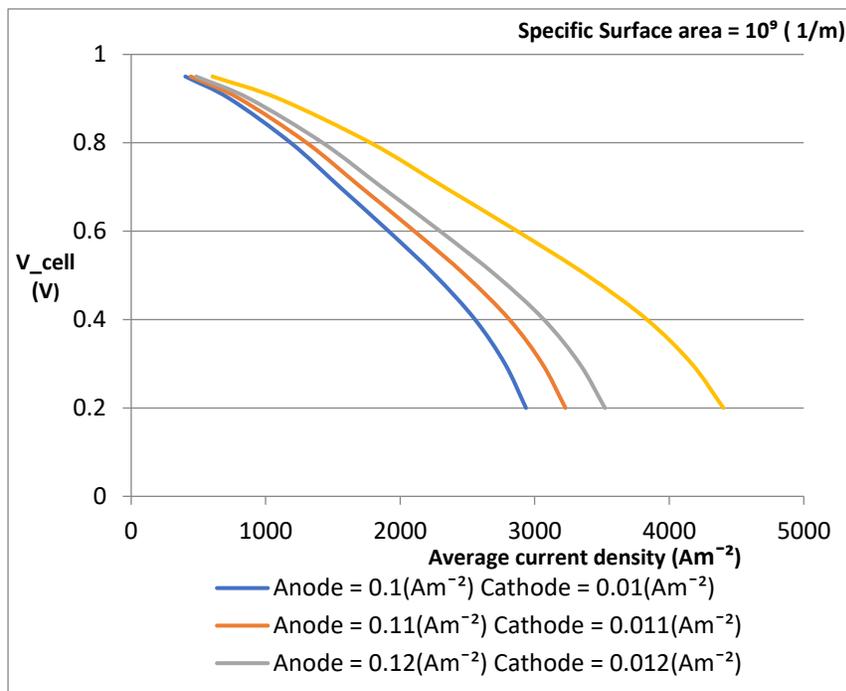
The power and the polarization characteristics of the cell were plotted at different specific surface areas. In the model, the specific surface area at the anode and the cathode was considered to be 10^9m^{-1} . The anode and the cathode current densities were changed. The power characteristics of the SOFC obtained were -

HIGH TEMPERATURE SOFC TO OPTIMIZE THE PERFORMANCE

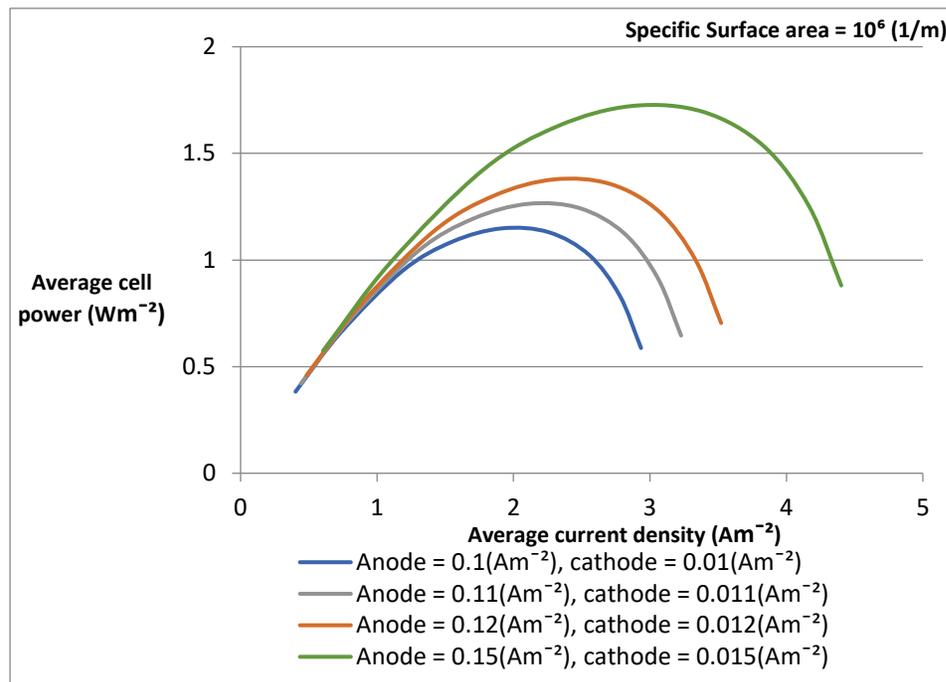


From the graphs, it is clear that as the exchange current density increases, the output power of the SOFC also increases. Even a slight change in the exchange current density brings a significant change in the output power.

Similar trends were seen in the polarization characteristics. The cell voltage increased with increase in the exchange current density.



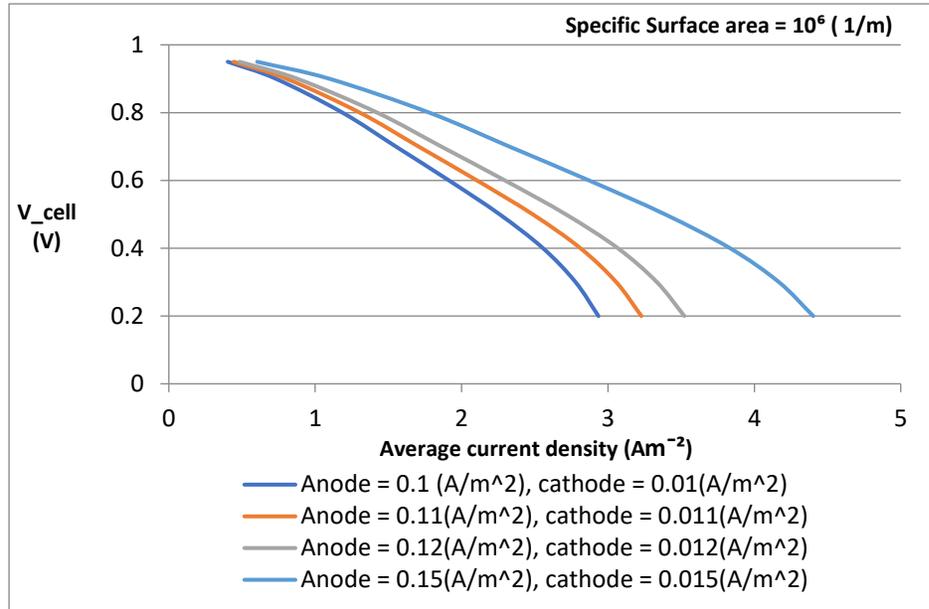
Then the same variation is also studied by changing the specific surface area of the anode and the cathode to 10^9m^{-1} (keeping operating temperature of SOFC at 800°C). The variations showed a similar trend but the magnitudes of the power output and the cell voltage changed (decreased) quite significantly. The power characteristics for the various values of exchange current density were obtained as follows.



From the graph it can be seen that as the specific surface area decreases, the average current density and the average cell power decrease. However increase in the exchange current density increases the average output power of the cell.

Similarly, the polarization characteristics of the cell obtained for the variation in the exchange current density are as follows.

HIGH TEMPERATURE SOFC TO OPTIMIZE THE PERFORMANCE



It is clear from the above, that as the specific surface area decreases, the average current density output of the cell for given cell voltage decreases drastically. However, increase in exchange current density of the anode and the cathode increase the cell voltage for a given exchange current density.

5. CONCLUSIONS

A parametric study of the single solid oxide fuel cell in planar configuration has been done using COMSOL Multiphysics (5.5.0.292) software. The Polarization characteristics and the power characteristics have been plotted for various changes in parameters like temperature, pressure, exchange current density, Kinetic volume of inert gas and electrolyte width. A significant effect of the variation of these parameters on the performance of SOFC has been observed and is discussed. The output power and the cell voltage at different operating conditions can be known from the model which helps to optimize the performance of fuel cell.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

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HIGH TEMPERATURE SOFC TO OPTIMIZE THE PERFORMANCE

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