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EVALUATING PERFORMANCE OF A SINGLE HIGH TEMPERATURE SOLID OXIDE FUEL CELL WITH PARAMETRIC SIMULATION OVER ITS DIMENSIONS

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Abstract: The versatility of fuel cells makes them the future of energy sources on Earth. In this paper, a three dimensional solid oxide fuel cell in planar configuration, with hydrogen fuel and air as oxidant, has been modeled using COMSOL Multiphysics software. The gas flow in the gas channels is modeled by Navier Stokes equations while that through the electrodes is studied by applying the Brinkman equations. The model is simulated for the variation in the sizes of the gas diffusion channel including length, height and width of the channel. The polarization and power characteristics of the cell are plotted and studied over the variations. The cell performance is evaluated considering counter-flow and co-flow of the gases in the channels, separately. A clear impact of the change in the sizes of the channel is observed on the performance of the cell. A comparison of the counter-flow and co- flow patterns has also been made.

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1. INTRODUCTION

The conventional energy sources are limited in amount on earth. So, continuous efforts are being put on by the scientific community to develop alternative and sustainable energy sources and put them into practical use. Solar devices seem promising but have their own limitations like inability to work in dark, require larger area, battery storage requirement etc. [1]. Moreover, the development and disposal of the semiconducting devices used in solar cells is not environmental friendly [2]. Fuel cells appear to be an apt solution of our future energy requirements. A fuel cell is an electrochemical device which converts the chemical energy of the fuel directly into the electrical energy i.e. the chemical energy is not converted to heat but instead direct electrical energy is obtained [3]. For the same reason, they have higher thermodynamic efficiency than the combustion engines. There are various types of the fuel cells under development viz. Alkaline Fuel Cell (AFC), Molten Carbonate Fuel Cell (MCFC), Polymer Electrolyte Membrane Fuel Cell (PEMFC), Phosphoric acid Fuel Cell (PAFC) and Solid Oxide fuel Cell (SOFC). The SOFCs are a preferred choice for their use in the electric power generation systems because of their easy handling, as the electrolyte used in SOFC is in solid state, and low cost. Moreover they generally operate at higher temperatures ($\sim 600\ ℃ - 1000\ ℃$), so hydrocarbons can be directly fed into the fuel cell and conversion of the hydrocarbon to hydrogen can take place inside the fuel cell itself [4, 5]. Further, a SOFC is not affected by the presence of carbon monoxide; instead it acts as a fuel for the SOFC [6]. Thus a SOFC is highly efficient and increased efficiency, up to 70%, has been reported in Integrated SOFC- combustion turbine pressurized power transmission systems [7, 8]. The working of a SOFC is based on the basic reaction of hydrogen combining with the oxygen to generate water and energy. Since water is the product formed, so a fuel cell is a clean source of energy. A SOFC is the most promising fuel cell system which can replace the traditional fossil fuel engines in power production systems. Several studies pertaining to the modeling and simulation of SOFCs have been made [9]. Some researchers [10] have focused on modeling a steady state 2-D SOFC in tubular configuration and have evaluated the voltage sensitivity over various parameters while some researchers [11-13] have modeled three dimensional SOFC and have analyzed the variation of fluid flow, using various fuels. But only a few studies have been reported in which the size optimization along with the flow pattern performance analysis has been made [14, 15]. This paper presents a 3-D steady state model of a single SOFC in planar configuration. The model is simulated for the various changes in the sizes of the fuel cell and the effect of change in the dimensions on the cell performance, with gas flow in counter-flow manner and co-flow manner, is studied.

2. MODEL OF SOFC

Modeling a SOFC requires inculcating several physical phenomena in the model. Certain assumptions are made to simplify the model, but at the same time the model must also be close to the real world situations. This paper attempts to model a three dimensional single SOFC in planar configuration on COMSOL Multiphysics® software.

(I) Assumptions

Following Assumptions have been made while modeling the fuel cell.

1. The gases are ideal gases i.e. the interaction between the molecules of the fuel and the oxidant are not considered. This can be considered as the temperature of the system is kept high ($\sim 800\ ^\circ\mathrm{C}$) and for high temperature the real gases behavior approaches to that of ideal gases.
2. The flow of gases in the flow channels is considered laminar flow.
3. The temperature of the fuel cell is assumed to be constant at 800 ℃.
4. Both anode and cathode are assumed to be isotropic and homogeneous.
5. The fuel is assumed to be humidified hydrogen, rather than a mixture of hydrocarbons, and the oxidant is considered to be humidified air.

(II) Structure of SOFC

A typical SOFC consists of an anode, a cathode and an electrolyte (in solid state). Considering the transport, a SOFC has two flow channels, one for the fuel and the other for the oxidant. The fuel channels are responsible for the distribution of the gases through the fuel cell, along the electrodes. The fuel channel is along the anode and serves two purposes. It brings the fuel (humidified hydrogen) for the fuel cell and removes the steam produced in the chemical reaction in the cell. The air channel, along the cathode, on the other hand has the oxidant (humidified air) and is not required to take out any gases out of the fuel cell. The model considers the flow of gases in the channels to be governed by compressed Navier Stokes Equation given below [16,17].

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

Here u is the 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 takes into account four basic forces on the fluid inside the fuel cell. The left hand side of equation i.e. $\rho\left(\frac{\partial u}{\partial t}+u.\nabla u\right)$ represents the inertial forces of the system, term $(\nabla \mathrm{p})$ represents the force exerted on the fluid by fluid pressure, viscous forces on the fluid are represented by $\nabla(\, \mu(\nabla \mathrm{u})+(\nabla \mathrm{u})^{\mathrm{T}})-\frac{2}{3}\, \mu\, (\nabla \mathrm{u})\, \mathrm{I}\,)$, while F corresponds to the external forces applied. The gas flows in the respective channels are due to slightly higher pressure drops at the inlets of cathode and the anode. In the model, pressure of 6 Pa is assumed at the cathode inlet and 2 Pa at anode inlet.

(III) Modeling Gas flow in electrodes

To model the gaseous flow in the gas diffusion electrodes, Brinkman Equations are considered to be the governing equations as they represent the combined effect of Navier Stokes Equations and Darcy’s Law [18]. The equation used is

$\nabla p = -\frac{\mu}{k}\, v + \mu_e \nabla^2(v)$, Here, μ represents the viscosity of the fluid, v is the velocity and μ_e is the effective viscosity parameter.

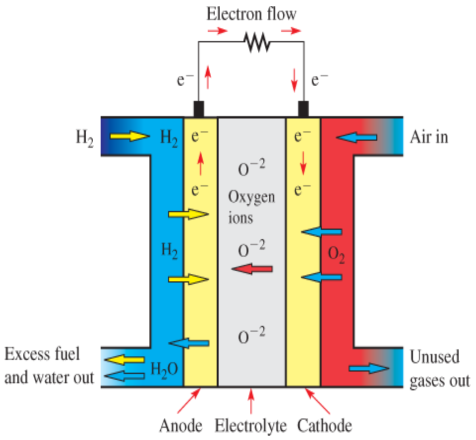
(IV) Materials chosen

The anode is made up of material having sufficient porosity to allow the flow of fuel through itself. Similarly the cathode is made up of a material which easily allows the flow of the oxygen ions, through itself, for oxidation of the fuel. Both the anode and cathode should be conducting. Cathode is considered to be made up of Lanthanum magnetite with Strontium doping while anode is considered to be made up of Nickel Oxide cermets. Yttrium Stabilized Zirconia (YSZ) is used as the electrolyte as it allows the flow of oxide ions through it. Anode, Cathode and the electrolyte are so chosen that they can withstand the high temperature of the fuel cell [19-23]. The oxygen from the oxidant (humidified air in this case) reacts with the metal cathode and forms oxide ions which diffuse through the porous cathode and through the electrolyte to reach the anode. At the anode they combine with hydrogen of the fuel and form water (steam). The formation of each water molecule liberates two electrons which flow towards the cathode through the outer circuit thus constituting the current [24]. The reactions taking place at anode and cathode are, respectively

$$2H_2 + 2O^{2-} \rightleftharpoons 2H_2O + 4e^-$$

$$O_2 + 4e^- \rightleftharpoons 2O^{2-}$$

The action of a fuel cell can be shown as below.



OPERATION OF SOFC [25]

(V) Modeling charge transfer

In this model, the charge transfer current density in the SOFC model has been studied by applying Butler Volmer charge transfer kinetic equations. The Butler Volmer equation [26], at the anode, 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 $i_{a,0}$ corresponds to the exchange current density (anode), c_{H_2} is the concentration of hydrogen, $c_{H_2,ref}$ is taken as the reference concentration of hydrogen, c_{H_2O} is the concentration of water vapours, $c_{H_2O,ref}$ is taken as the reference concentration of water vapours, F is the Faraday's constant, T is the absolute temperature, R is universal gas constant, and η is the overvoltage.

Similarly, at the cathode, the Butler Volmer charge transfer kinetic equation is

$i_{ct,c} = i_{c,0}\left(\exp\left(\frac{3.5F}{RT}\eta\right)-n_{O_2}\frac{c_t}{c_{O_2,ref}}\exp\left(\frac{-0.5F}{RT}\eta\right)\right)$, Here $i_{c,0}$ is the exchange current density (cathode), c_t is the total concentration of the species and n_{O_2} is the molar fraction of oxygen.

The overvoltage η, in the SOFC, is defined as

$\eta = V - V_{equil.}$, Here $V_{equil.}$ represents the equilibrium potential difference and V is the electrode potential. All the terms in the above equations are taken in SI system of units. The electrons move from lower potential to higher potential i.e. the anode is at lower potential, as the electrons move from anode to cathode in the outer circuit. So, to find cell voltage, the potential at the inlet of anode is taken to be zero (as a reference) and at the cathode inlet boundary is taken to be equal to cell voltage V_{cell}. One can define the cell voltage as

$V_{cell} = \left(\left(V_{equil.}\right)_{cathode} - \left(V_{equil.}\right)_{anode}\right) - V_{pol}$, Here, V_{pol} represents the voltage losses inside the fuel cell due to irreversible processes and is called polarization voltage. It consists of three major components viz. Ohmic polarization V_0 (due to resistance of various parts of fuel cell), Activation polarization V_{act} (owing to resistance to reaction at the electrode surfaces) and Concentration polarization V_{conc} (taking into account the change in the concentration of fuel and the oxidant as they propagate in their respective channels). Thus $V_{pol} = V_0 + V_{act} + V_{conc}$.

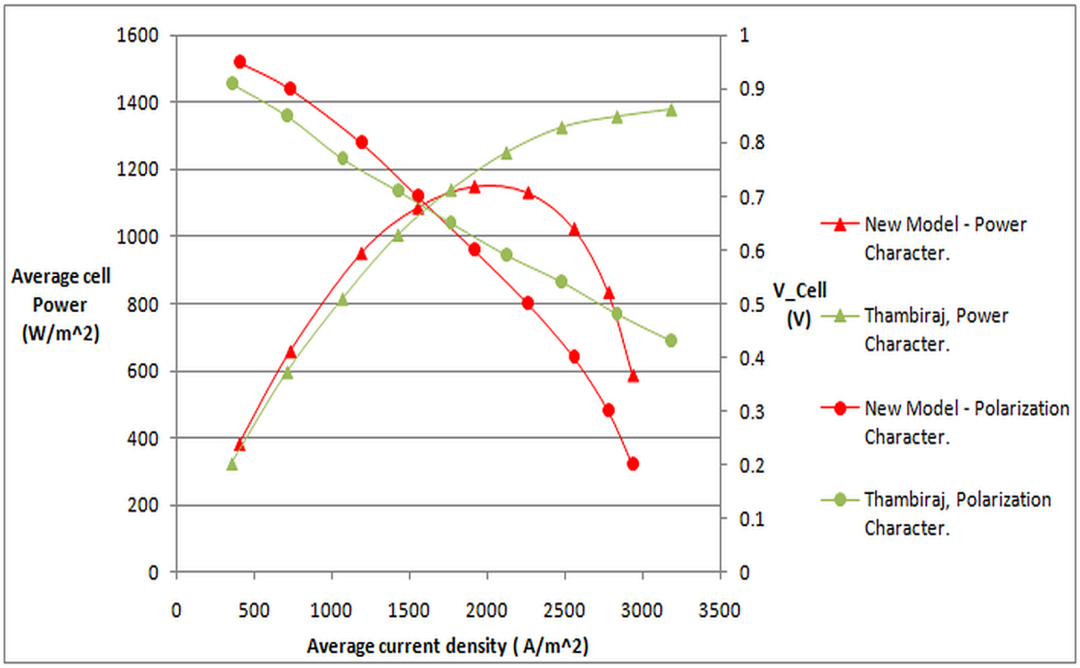
The model considers $\left(V_{equil.}\right)_{anode} = 0$, $\left(V_{equil.}\right)_{cathode} = 1\,V$ and V_{pol} is varied from 0.05 V to 0.80 V thus obtaining the cell voltage ranging between 0.95 V and 0.20 V respectively. The ionic and the electronic charge balances are studied by applying Ohm's law. All the external boundaries of the fuel cell are considered to be insulating i.e. zero mass flux is considered. The gas flow in the respective channels and the electrode is considered to be in accordance with the Maxwell Stefan distribution. However, at the outlet, the gaseous flow is considered due to convection only.

(VI) Multiphysics Modeling

Considering the above physical processes, a 3D model of a single SOFC in planar configuration has been developed on COMSOL multiphysics software [25]. In the model, the channel height, channel width and rib width were assumed to be 0.5 mm each while the channel length was considered to be 1 cm. The thickness of diffusion electrodes is considered 0.05 mm, for anode as well as cathode. The SOFC model was simulated for the various changes in the sizes of channel. In the simulation, the temperature of the SOFC was assumed to be constant at 800℃. The model was simulated for counter-flow (oxidant and fuel move relatively in opposite directions in their respective channels) and co-flow (oxidant and fuel move relatively in same direction in their respective channels).

3. MODEL VALIDATION

The polarization and the power characteristics are plotted for the model and compared with the results of the experiments carried by N. Thambiraj et al. for the operating temperature at 800℃. The model results are in good agreement with the experimental results and the general trend, in both polarization and power characteristics is similar [27].



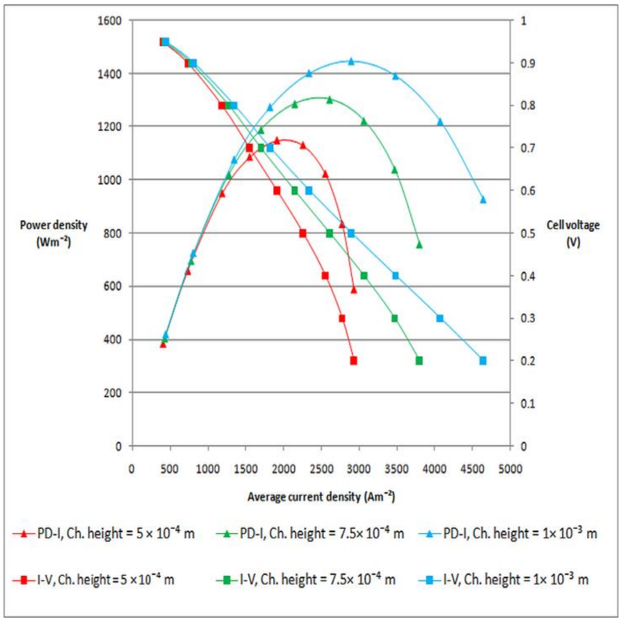
Model Validation

This model gives slightly higher power at lower values of current density as compared to Thambiraj et al. model. The difference in the power density and the cell voltage at higher current densities is due to different composition of fuel considered in the Thambiraj et al. model. They have considered the fuel to be a mixture of CO_2 and hydrogen in such a proportion that the depletion of fuel is avoided at higher current densities, consequently, higher cell voltage is observed. However the trend obtained in the present model is similar to that reported in literature [11].

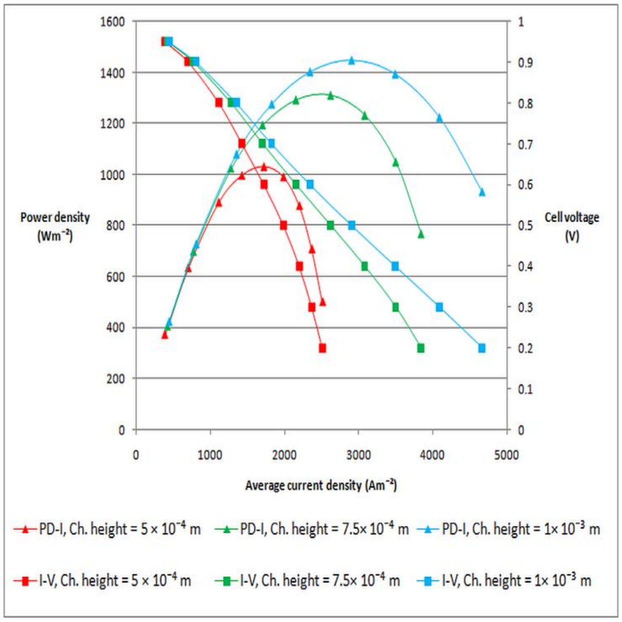
4. RESULTS AND DISCUSSION

(I) Variation in Channel Height

Considering the temperature of SOFC to be 800 ℃, the channel height is changed to 0.75 mm and to 1 mm from 0.5 mm, for simulating the model to analyze the polarization and the power characteristics. The model is simulated for both the counter-flow and the co- flow of the gases.



(a) counterflow characteristics

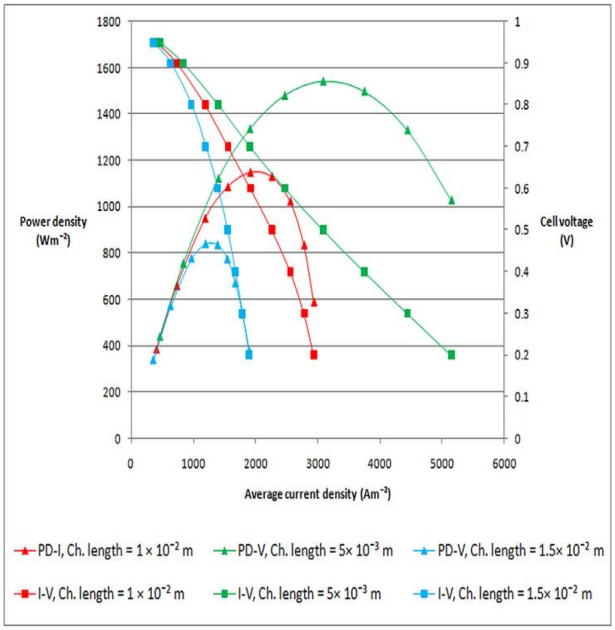


(b) co-flow characteristics

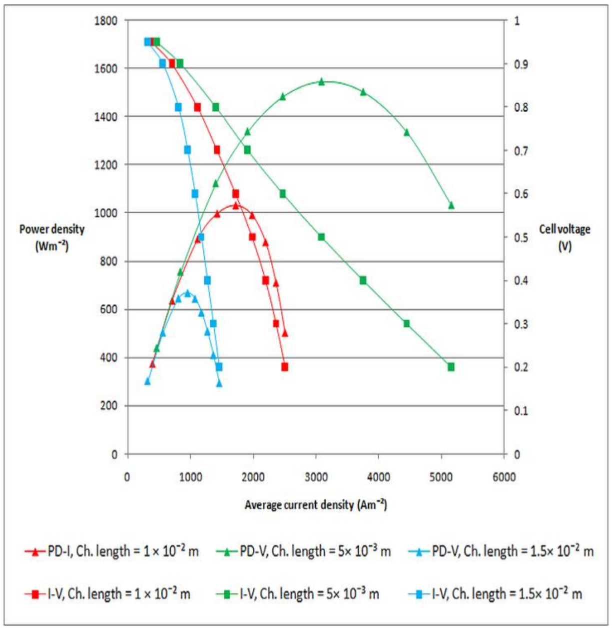
The maximum power output of the SOFC shows an increase with increase in channel height for both counterflow and co-flow. Also, the maximum power output is obtained at higher current density as the channel height is increased. A comparison of the characteristics in counter- flow and co-flow pattern indicates that the power output is more in counter- flow pattern as compared to co-flow at small channel height, but as the channel height increased to 1 mm, a slightly higher peak power density was observed in co-flow pattern. The increase in the power density and the cell voltage with increasing channel height might be due to the decreased speed of the gas in more volume of channel and thus the gas gets more time for diffusion through the electrode.

(II) Variation in Channel length

The SOFC model was simulated for the changes in the length of the channel for both counter-flow and co-flow of the gases. The channel length was initially kept at 0.01 m and both increase and decrease in length of the channel were simulated and polarization and power characteristics were plotted.



(a) counterflow characteristics

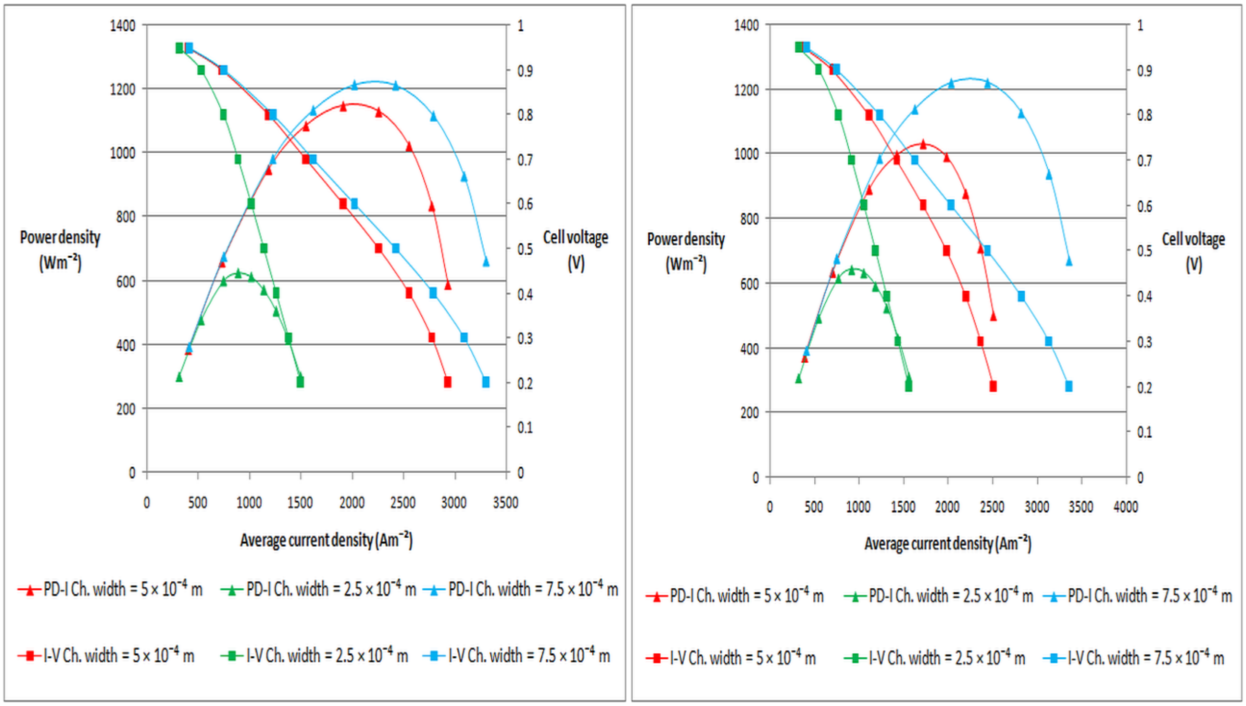


(b) co-flow characteristics

The simulation shows that SOFCs with longer channel lengths have lower power output. The effect is more pronounced for co-flow as compared to counter-flow pattern. The current density for the maximum power output shows an increase with the decrease in the length of the flow channels. The power output and cell voltage in co-flow are less than the corresponding values in counter- flow of gases for longer lengths of the channels. However as the channel length decreases the performance of the cell in co-flow approaches to that in the counter-flow pattern. This trend might be due to the increase in pressure of the gas inside the channel, with decreasing channel length, hence making it easy for the gas to pass through the electrode hence increasing the cell voltage and consequently the power output.

(III) Variation in Channel Width

The simulation was performed for the model for various channel widths (keeping other dimensions of the cell as constant). Assuming the initial channel width in the model to be 5×10^{-4} m, both increase and decrease in the width were simulated in counter and co-flow of the gases in channels.



(a) counterflow characteristics (b) co-flow characteristics

It is clear from the simulation results that an increase in channel width increases the cell voltage for a given current density and hence power output also increases. Also, with increasing channel width, the output cell voltage is obtained at higher current densities thus shifting the maximum power output towards higher current densities. The variation is similar to that observed when the channel height is changed. The maximum power obtained in the counter-flow is more than that in co-flow pattern at channel width of 0.5 mm. But, as the channel width increased, more power is developed in the co-flow of the gases as compared to the counter-flow.

5. CONCLUSIONS

The simulation results indicate that the maximum power output of the SOFC increases with decreasing channel length, increasing channel height and increasing channel width. The patterns obtained are similar in counter-flow and co-flow of gases. Initially, in the model, the counter-flow pattern gave better output power than co-flow but as the model was simulated for the changes in sizes, for higher values of power density, the counter-flow and co-flow patterns approached each other.

As the power output increases, the peak of the power characteristics also shifts to higher values of current densities. The same results should be validated experimentally to optimize the size of the fuel cell for maximum output.

CONFLICT OF INTERESTS

The author(s) declare that there is no conflict of interests.

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