



# A Numerical Study On Current density & Power Density For Nanostructured Thin Film Solid Oxide Fuel Cell

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## Abstract

The present method for improving the thermal performance [24] & efficiency of traditional [24] materials and mono-nanomaterials involves adding a variety of nanoparticles to the base material [24]. The purpose of the present study is to carry out a numerical analysis of recent advancements [1] in power density with YSZ [11] (Yttria stabilised zirconia) nanomaterial thin films as anode and cathode materials. From this study it is found that power density for YSZ (Yttria stabilized zirconia) nanomaterial is  $1351 \text{ W/m}^2$  at temperature of 600K. From this study, we conclude that for operating temperature range from 600K - 800 K, all the Polarization losses like (Activation losses, ohmic losses & concentration losses) which are present at the interface layer between anode and electrolyte decreases. Therefore, the value for Current density & power density increases. YSZ nanomaterial thin film significantly enhances the solid oxide fuel cell efficiency [21]. The author hopes that their study will benefit current researchers and practitioners active [12] in the Sofc [12] in addressing the challenges to increase power density and current density for automotive applications and will also be useful in dealing with solid oxide fuel cell [14] difficulties in a meaningful manner.

## Keywords

Nanostructured thin film , numerical data , solid oxide fuel cell , Cell power , current density

## Introduction

Researchers are continuously trying to create new materials that would be focused on effective heat and mass transport [25] systems. Therefore numerous scientists [25] & researchers [25] established that nanomaterials, as opposed to bulk materials, would improve the system's thermal performance [25]. Nanomaterials are synthetic colloids made of a base substance and nanoparticles (1–100 nm). Experts are still looking into the mysterious properties of nanomaterial. TiO<sub>2</sub> nanomaterial has superior thermal transport characteristics than distilled water, according to

recent research by Sajid et al. (2019) that involved experimentally varying TiO<sub>2</sub> nanomaterial concentrations. Gopal et al. (2020) [1] examined how temperature variation [1] and heat generation/absorption affected [1] nanomaterial over a permeable cylinder [1] and found that it's preferable to include flow measure for curvature [1] to enhance friction [1]. Upadhyaya et.al (2020) [1] studied the thermal exchange [1] properties of a graphene nanofluid [1] using water and ethylene glycol as the base fluids. In comparison to water-based graphene nanomaterial, they found that Greater heat transmission is demonstrated by graphene nanofluid based on ethylene glycol [1]. The Magnesium oxide nanoparticles' effects [1] on irregular boundary layer flow [1] was investigated by Raju et.al (2019), who discovered that increasing the irregular convection parameter [25] increases the thermal exchange.[14]

Nanoscience is the most recent technology or methodology we employ today for various purposes. Today, we will only be focusing on nanotechnology's role in fuel cells among other applications. The benefit of fuel cells is their high electrical efficiency [20] and fuel flexibility over other devices since they are typically used to convert fuel to electricity through an electrolytic process (redox reaction). Here, we'll talk about solid oxide fuel cells. We'll present and talk about different kinds of nanomaterials that are useful for fuel cells in the automobile industry.[9]

One of the most efficient fuel-cell [24] technologies is the solid oxide fuel cell [24] working at maximum functioning temperatures from 800°C-1000°C with high efficiency. In this literature review table we have discussed the fundamental elements of a SOFC are like (anode, cathode, electrolyte, and connector), Various types & their characteristics. Abdalla M. Abdalla et.al (2018) focused majorly focus on this type of fuel cell & its performance. They are majorly focused on a combination of nanomaterials at different operating temperatures and calculated the performance at varying temperature ranges. Similarly, N.Alhazmi et.al (2021) discussed about button-type solid oxide fuel cell, as their major focus is on different temperature ranges at which solid oxide fuel works so they developed a 3D cad model for SOFC and compared the results for performances at varying temperatures.

Figure 1 shows the schematic diagram for Sofc.

Basically it consists of three porcelain layers: one solid electrolyte and two porous electrodes, Major Material properties for sofc fuel cell covers [1]-

1. Electrical conductivity
2. Thermal stability
3. Catalytic activity
4. Chemical stability
5. Power density

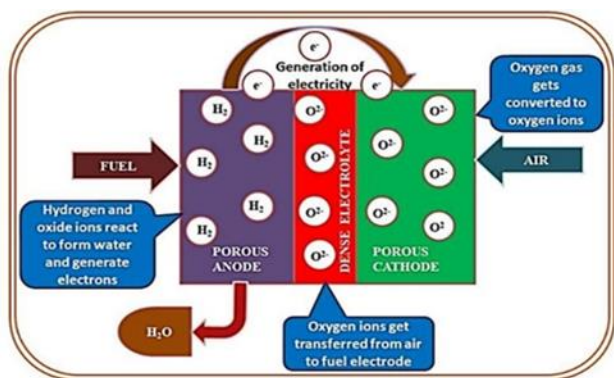


Fig 1. Solid oxide fuel cell

Given table no 1, shows the metal-based nanomaterial for anode, cathode and electrolyte which we have used for our study and simulation

Table 1

SR. NO	Components	General used material
1	ANODE	Ni –YSZ doped cermet or GDC used due to its high electrical conductivity and stability at different temperature
2	CATHODE	Strontium doped La MnO <sub>3</sub> or lanthanum manganite doped with rare earth elements
3	ELECTROLYTE LAYER	YSZ (Yttria stabilized zirconia) or zirconium oxide stabilized with yttrium oxide is used as a ceramic material

## 2. Literature study

2.1 Abdalla M. Abdalla on Nanomaterials for solid oxide fuel cells: A review (et.al). [3]

In this paper, Abdalla and his team focused on solid oxide fuel cell [3] & its performance. They are majorly focused on a combination of nanomaterials at different operating temperatures. As considering that the cell working temperature is important [5] for enhancing the effectiveness of fuel cell. Hence, following table shows the various combination of nanomaterial used for electrolytes and electrodes at different temperatures.

Table 2 [3]

ANODE [3]	CATHODE [3]	ELECTROLYTE [3]	TEMPERATURE (Å°c)
Ni	Pt	Gdc [3]	450-550[3]
Ni [3]	Lsm-Ysz	Scsz (Scandia Stabilized Zirconia) [3]	700[3]
-	Lscf-Gdc [3]	Gdc [3]	650-850[3]
Pt [3]	Lscf [3]	Ysz (Ytria Stabilized Zirconia) [3]	450-500[3]
Ni-Sdc [3]	Ssc [3]	Scsz [3]	600-700[3]
Ru [3]	Pt [3]	Cgo-Ysz [3]	470-520 [3]
Pt [3]	Pt [3]	Ysz [3]	350-500[3]
Ni [3]	Pt [3]	Ysz [3]	600[3]
Pt [3]	Lscf [3]	Ysz [3]	400-500[3]
Pt- Zro2 [3]	Lsm [3]	Ysz [3]	650-800[3]
Lscf [3]	Lscf [3]	Cgo [3]	700[3]
Psm [3]	Psm [3]	Ysz [3]	500-800 [3]
Ssc-Nio-Ysz [3]	Ssc-Lsf-Gdc [3]	Ysz [3]	700-800 [3]

2.2 N. Alhazmi on Three-dimensional computational fluid dynamics modeling of button solid oxide fuel cell (et.al) [13,20]

In this paper, N.alhazmi and their team have discussed button-type fuel cells. They have developed a 3D analytical model for fuel cell using Gambit software and further simulated & plotted results for temperature vs current density and voltage vs current density using Ansys fluent software. In their study, they used different material properties & boundary conditions to simulate the results using CFD (Fluent) software and finally they have concluded their results using a plotted graph. In their study after using the major input parameters like cell voltage 0.6v, oxygen flow rate 0.4 L min<sup>-1</sup> [13], and hydrogen flow rate 1.2 L min<sup>-1</sup> [13] for three varying temperature range [13]. The desired results indicate that when the temperature increased from 973 K [13] to 1023 K [13] to 1073 K [22], the fuel cells' current density [13] increased from 455.6 to 935.2 mA cm<sup>2</sup> [13]. Figure 2 shows that when temperature increases from 973K to 1023K, current density value also increased which is indicated by Red colour. And figure 3 shows the plot for current density vs temperature.

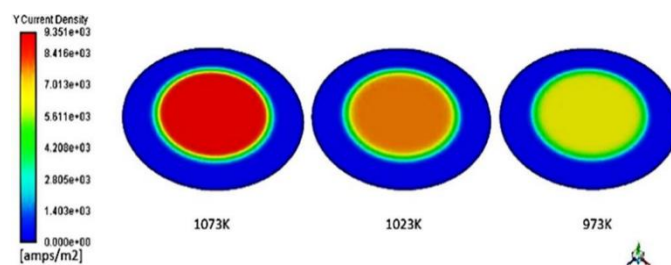


Fig 2 temperature distribution vs current density [22]

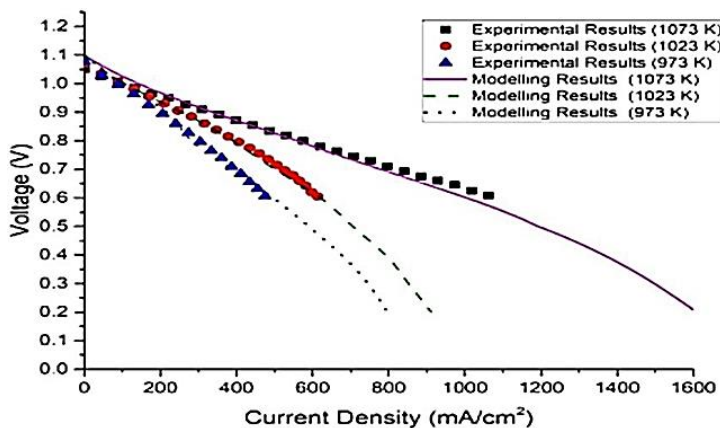


Fig 3. current density vs voltage [22]

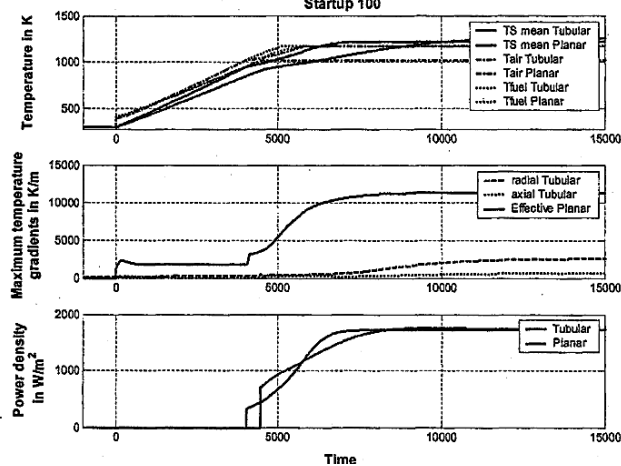


Fig 4. Startup performance for fuel cell

2.3. Miriam Kemm , Bjorn thorud on Planar And Tubular Solid Oxide Fuel Cells: A Comparison Of Transient Process Behavior (et.al) [6, 28]

In this paper, they have discussed and compared two major types of solid oxide fuel cells (SOFC), which are tubular counterflow types sofc and planar crossflow type sofc. Though they have used similar boundary conditions, electrochemistry, material properties and varying geometrical parameters for both models. Here, by simulating load [28] variations, start-up [28] and shut-down [28] operations, the transient behaviour of the planar [28] and tubular cell [28] geometries has been [28] calculated. Their major goal is to estimate & compare the result's power density , startup time and shutdown time using different geometry. Hence the desired results indicate that despite having similar flow areas the heat-up duration time taken by the tubular is 1 hour, while for planar is 1 hour 15 minutes, which means the startup time for planar is more than tubular. In case of power density as temperature increases , power density for planar model slightly gets increases as compare to tubular model [6]. Figure 4 also indicate performance of the fuel cell's start-up time [6] w.r.t temperature , power density [6]

2.4 M Saied on Investigations of solid oxide fuel cells with functionally graded electrodes for high performance and safe thermal stress (et.al) [30]

In this paper, they have discussed the effectiveness and thermal variation for a solid oxide fuel cell with functionally graded electrode using a (ni-ysz-ysz-lsm) type of combination of nanomaterial for electrodes and electrolytes. In their study, they have developed a 3D cad model using cfd software considering various governing equations, boundary conditions and material properties and at different grading parameter. Further, they have simulated the result for voltage (V) and cell power (W/m<sup>2</sup>). The result shows when voltage increases upto value 0.6 V [30], power density also gets increases by 23 percent [30] for functional graded electrode parameter 'm' [30]. Figure 5 indicated the when 'm' value increases from 0 to 2.0, Current density value also gets improved and at value 2.0 for 'm' they achieved high power density [30]. Also figure 6, shows similarly results for power density as 'm' value increases , power density also increases.

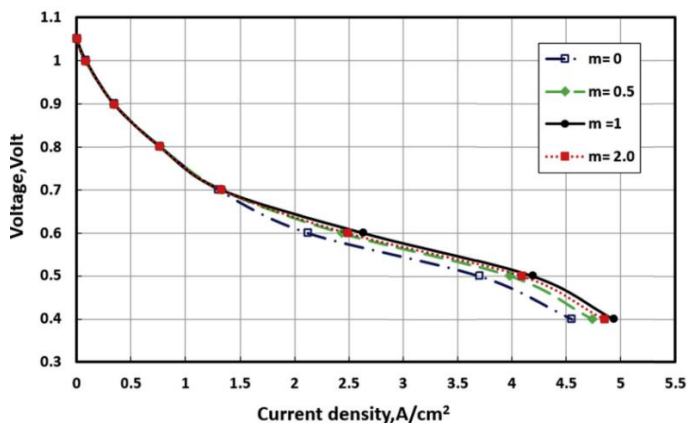


Fig 5. Current density VS voltage [30]

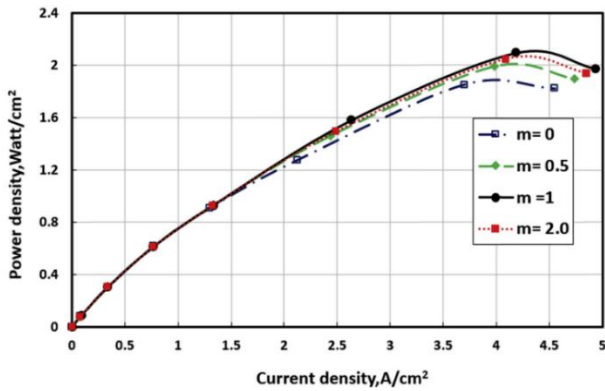
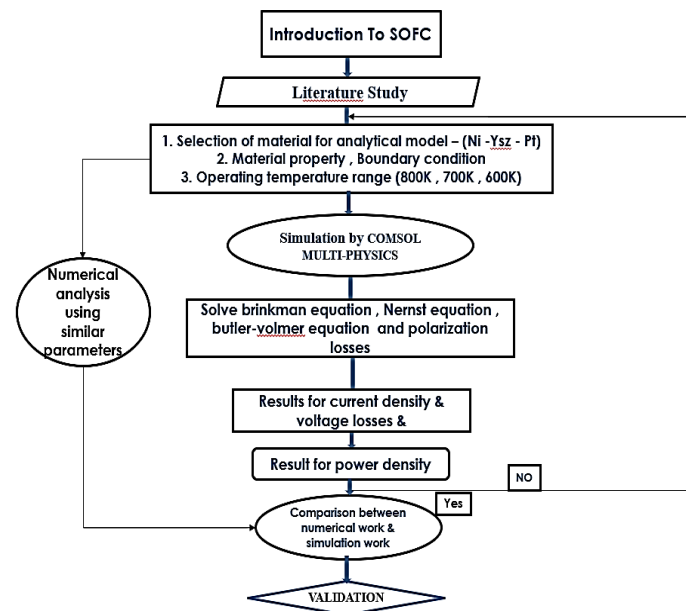


Fig 6. Current density vs power density

### 3. Research Methodology

In this study as our major focus is to achieve high power density for Solid oxide fuel cell at low temperature 600K, So to achieve this goal we have gone through systematic procedure like firstly we have done literature study on (sofc) to understand the electrochemistry, working principle for fuel cell, we have also studied about various kind governing equation & nanomaterial which are used for developing sofc. After this we have selected a set of nanomaterial which is (Ni-ysz-pt) and temperature range from 800k to 600k. Further we have developed a 3D analytical model using comsol mutliphysics software and simulated the results for current density & power density for varying temperature range. In order to achieve highest power density we repeat the procedure for temperature range 800 K to 600 K.



### 4. Numerical Model For Sofc

In this study, we built the model & simulate the results for

nanostructured Solid oxide fuel cell in 2D and 3D while taking into account a number of design factors and operational requirements [13]. By the literature study, We knew that Sofc works at high operating temperature specifically at 800°C, but at a high-temperature range we get a Polarization losses like (Activation, ohmic, and concentration polarization). This lowers the fuel cell's system performance, Hence here, we are designing a 3D cad model for nanostructured planar sofc [9] and generate simulation results for power density (W/m<sup>2</sup>) [14] with respect to cell voltage (V<sub>cell</sub>).

This model includes the following [5] physics:

- Ionic and electronic charge balance [5].
- Butler-Volmer charge transfer kinetics [5].
- Distribution of flow in gas channels [5].
- Flow in the porous GDEs [5].
- Gaseous phase mass balances in gas [5] channels and porous electrodes [5].

By using the above given governing equation and laws we can calculate the plotted results for power density and polarization curves.

#### 4.1 Sofc Fuel Cell Geometrical Parameters

Sr.no	Parameters	Values
1	Gas flow channel width [8]	1e-3[m] [8]
2	Gas diffusion electrode thickness [8]	5e-5[m]
3	Electrolyte thickness [15]	1e-5[m] [22]
4	Gas flow channel height [22]	0.001[m] [22]
5	flow channel length [22]	0.019[m]

Table 3

#### Sofc Model Nomenclature

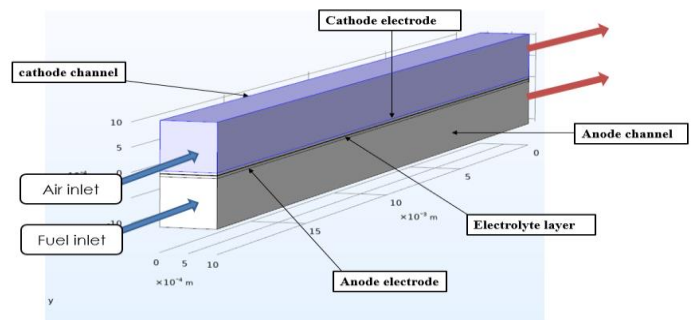


Figure 7. SOFC model nomenclature



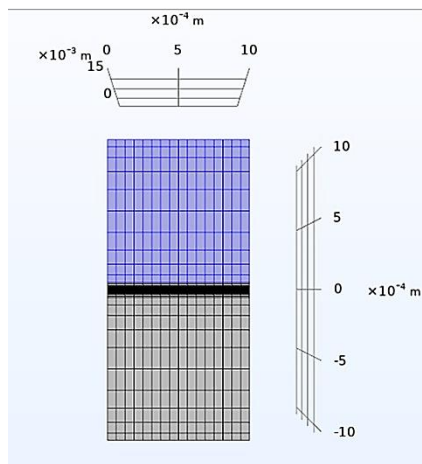


Figure 8. SOFC model Side view

### 3.2 Boudary Conditions

Table 4 (General boundary condition ) -

Sr.no	Parameters	Value
1	Inlet Mass flow rate	Anode = fuel (H2) , Cathode = Air (O2)
2	Pressure Drop	Anode = 2 Pa , Cathode = 5 Pa
3	Operating temperature at anode & cathode channel	600 k – 800 k
4	Atmospheric pressure at air and fuel exit [13] .	Zero
5	Walls have a no-slip boundary criterion [2]	$P = 0 \partial\Omega_{walls}$ [2]
6	Inlet Mass fraction	
	Oxygen (O2)	0.15
	Hydrogen ( H2)	0.4
	H2O	0.37
7	Reference concentration	
	C_o2ref	1.2559
	C_h2ref	9.7336
	C_h2oref	1.6223

### 3.3 . Electrical Properties Boundary Conditions

1. At the electrode and electrolyte boundaries, there may be electrical insulation or no flux. [13]

$$n \cdot (\nabla\phi) = 0 \quad (1)$$

2. At the anode's current collector, there is a designated electric

ground.[13]

$$\phi_e = 0 \quad (2)$$

3. Electric potential provided at the cathode's current collector [13]

$$\phi_e = V_{cell} \quad (3)$$

4. The electrochemical process at the electrode-electrolyte contacts causes a current density [13].

5. There is no flux set at the channel walls [13].

$$n \cdot J_i |_{\partial\Omega_{wall}} = 0 \quad (5)$$

Table 5 (electrical properties based pn material selection )

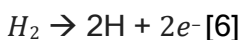
Sr.no	Parameters used	Values
1	Exchange current density, Anode [11]	0.52[A/m <sup>2</sup> ] [27]
2	Exchange current density, Cathode [27]	0.23[A/m <sup>2</sup> ] [27]
3	Viscosity	3e-5[Pa*s]
4	Permeability for (Anode, Cathode)	1e-10[m <sup>2</sup> ] [8]
5	Porosity	0.4
6	Effective conductivity for (anode , cathode ) [8]	1[S/m] [8]
7	Reference diffusivity [18]	3.16e-8[m <sup>2</sup> /s] [11]
8	Standard potential value (E°)	1.23
9	Equilibrium voltage, anode [17]	0(V) [17]
10	Equilibrium voltage, cathode [17]	1(V) [17]
11	Electrolyte thickness	1e-4[m]

### 3.6. Thermodynamics And Governing Equations For Sofc

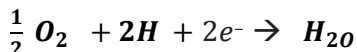
Working- In a fuel cell, an electrolyte is surrounded by an anode and a cathode. In this anode receives hydrogen gas [16] while the cathode receives [16] oxygen. The hydrogen [16] molecules are split by a catalyst at the anode into protons and electrons, which proceed in different directions to the cathode., A flow of electricity is produced by these electrons passing through an external circuit. When the protons reach the cathode through the electrolyte, they combine with oxygen and electrons to create heat and water.

The redox reaction for fuel cell can be given as [18].:

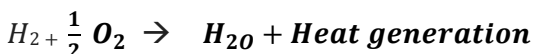
Anode :



Cathode :



Overall reaction



### 3.6.1 Nernst Voltage ( $E_{in}$ )

It is relation between equilibrium potential and operating anode potential, temperature and concentration of reactant and product. The given Nernst equation below formulae used to determine the Ideal voltage across the stack of cells

$$E_{nernst} = E^\circ_{nernst} + \frac{RT}{nf} \ln \left( \frac{CH_{2in}}{CH_{2Oin}} \right) \quad (9)$$

Where, E is the operating anode potential after deducting the voltage drop [4] brought on by internal resistance to a cell's optimal potential [4], whereas  $E^\circ$  is the equilibrium potential [4], R is the universal gas constant [4], T is the temperature in degrees Kelvin [4], and CH stands for the product reference concentration divided by the reactant reference concentration [4] and n is the number of moles given[4].

### 3.6.2 Butler-Volmer Equation

It is an equation that shows the electrode potential and current density relationship. It is used to calculate the current density [18] at the interface [22] by using the correlation of exchange current density [23], Where  $i_0$  = exchange current density [23],  $\alpha_a$  = charge transfer coefficient anode,  $\alpha_c$  = charge transfer coefficient,  $\eta_{act}$  = activation polarization and R = gas constant

$$i = i_0 \left\{ \exp\left(\frac{\alpha_n f}{RT} \eta_{act}\right) - \exp\left(\frac{(\alpha-1)nf}{RT} \eta_{act}\right) \right\} \quad (10)$$

### 3.6.3 Voltage Losses

Voltage loss is an important parameter to identify the actual performance of the fuel cell, the voltage at which sofc is working is always less than Nernst voltage which happens due to voltage loss. Therefore the above given Equation 10 is used to calculate actual losses, using the terms activation polarisation [2], ohmic polarisation [2], and concentration polarisation [2]. Hence, the operating voltage can be written as [2]

$$(V_{cell} = E - \eta_{act} - \eta_{ohmic} - \eta_{conc}) \quad (11) \quad (\text{Where}),$$

#### (i) Activation Polarization ( $\eta_{act}$ )

Activation losses are triggered by fixed rates of the electrochemical process taking place at the anode and cathode [2]. The equation for activation loss [2] can be given as.

$$\eta_{act} = \frac{2RT}{nf} \sinh h - \left(\frac{i}{2i_0}\right) \quad (12)$$

#### (ii) Ohmic Polarization ( $\eta_{ohmic}$ )

The fuel cell's resistance to charge transmission causes ohmic losses [2]. As these losses [2] happen across all three levels [2], but the electrolyte frequently experiences losses that are orders of greater magnitude [2].

$$\eta_{ohmic} = i * \left(\frac{l_{electrode}}{\sigma_{ionic}}\right) = i * R_{ionic} \quad (13)$$

#### (iii) Concentration losses ( $\eta_{conc}$ )

Concentration losses also referred to as mass transfer losses [2], are brought on by reagent reduction and product accumulation [2] inside the electrodes [2]. The effective diffusivity is represented by  $D_{eff}$ , the limiting current density is represented by  $i_L$ , and the proportion of reactant in the fuel or air channel is [2] represented by  $C_{k,channel}$  [2].

$$\eta_{conc} = \frac{RT}{nf} \ln \left( \frac{i_L}{i_L - i} \right) \quad (14)$$

## 4. Meshing For Fuel Cell Geometry

After designing the 3-D fuelcell model in COMSOL, Moving towards towards step postprocessing, in this we have generated fine quality mesh for this 3D model. The number of nodes at the respective electrode [2] and electrolyte [2] and channels [2] is specified to determine mesh density [13], which was achieved using a mapped mesh that we used [13]. In meshing result, we have generated Hexahedra mesh at channel's face, value for mesh vertices is (10920), no of element generated at channel face is (92800), which shows we have generated fine mesh, mesh volume is  $8.0e - 9 \text{ m}^2$

The mesh distribution has shown below –

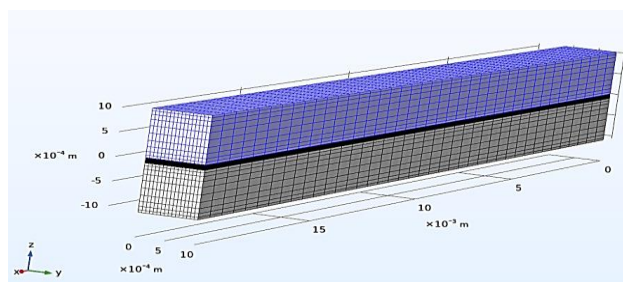


Figure 9. Meshing

## 5. Result & Discussion

### A). Cathode passage for oxygen mole fraction

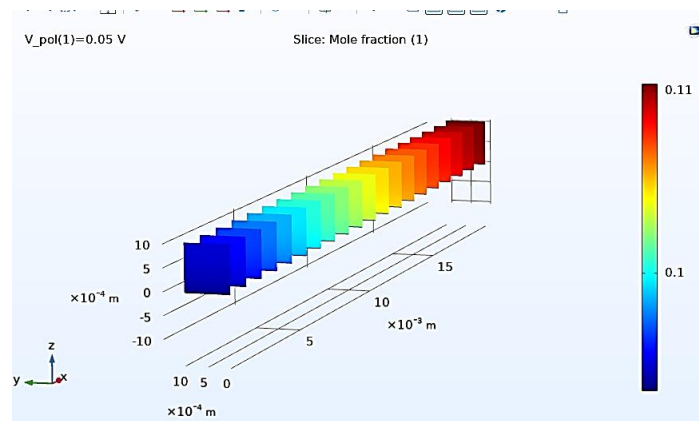


Figure 10. Oxygen Distribution

### B). Anode passage for hydrogen mole fraction

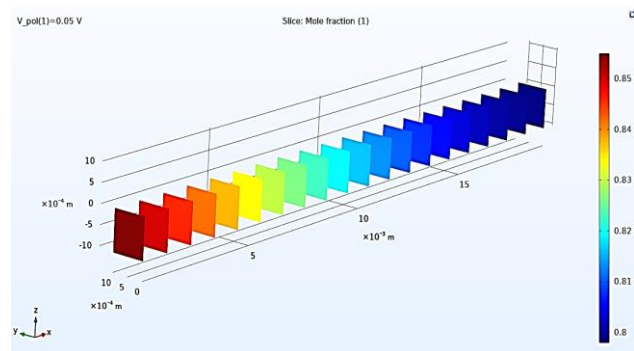


Figure 11. Hydrogen Distribution

### C). Current density distribution at a given cell voltage

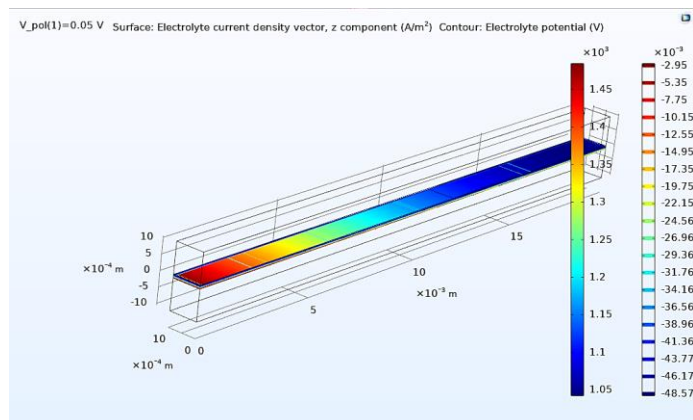


Figure 11. current density representation

### D). Average Current density vs $V_{pol}$

Figure 12 shows effect on the current density of polarization voltage with respect to temperature. By observation when we decrease the temperature from 800k to 600k, overall polarization losses will get decreases therefore we get maximum current density at 600K operating temperature which is around  $3650 \text{ A/m}^2$

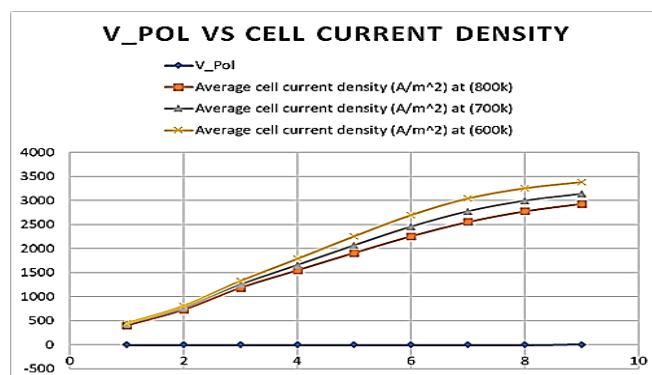


Figure 12. effect on current density of polarization voltage

### E). Polarization curve

Polarization curve is a curve which shows the changes in values of cell voltage (V) vs cell current density (I), as it is a direct relationship between current and voltage and if results for curve shows high current density at high voltage, It means we can have high power density. Figure 12 shows the Result and comparison for polarization curve at decreasing temperature range from (800k to 600k), we can observe that as temperature decreases from (800 to 600), polarization losses reduces & current density value gets increases with increase in cell voltage, hence at 600 k temperature we gets highest current density value which is  $3500 \text{ A/m}^2$  at 0.2v cell voltage.

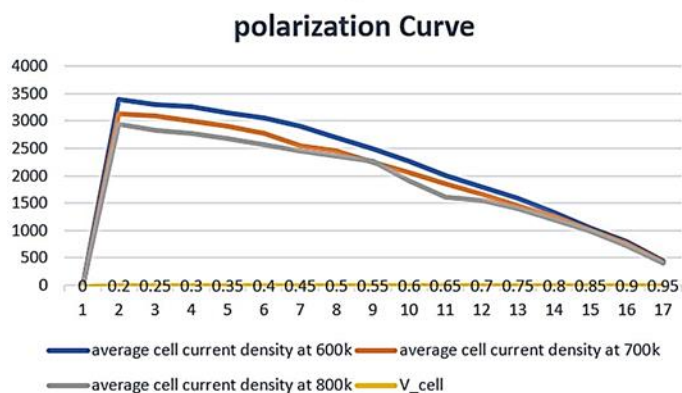


Figure 13. effect on current density for  $V_{cell}$

**F). Power density**

Figure 8. effect of power density for temperature range. Power density is rate of watt which we can get from a unit cell or we can also that how much cell power we can draw out of a unit cell. As we have observed in above results that for polarization curve & average cell current density we got optimized results at decreasing operating temperature. Similarly for power density results, when we move towards decreasing temperature (800 K to 600 K), polarization losses decreases. Hence at temperature 600 K. we got the highest power density value  $1351 \text{ W/m}^2$  with respect to average cell current density

Whereas , Power density =  $V_{cell} * I_{cell}$

Sr.no	Temperature ( $^{\circ}k$ )	Power density ( $\text{W/m}^2$ )
1	800	1149
2	700	1248
3	600	1351

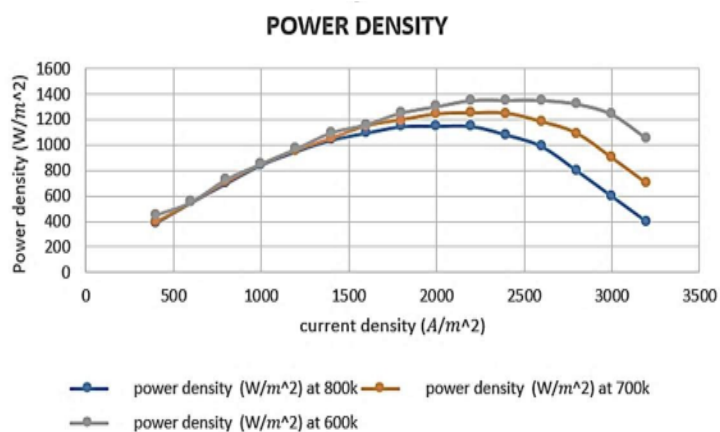


Figure 14. effect of power density for temperature range

**E). Validation**

By simulating the performance for solid oxide fuel cell at varying temperature range 800 K to 600 K , we observe that for simulation results we get highest value for power density at 600K temperature which is  $1315 \text{ W/m}^2$ . Now For validating the results for power density we have compared the simulation results with numerical results at same operating temperature 600K and same parameter. Through numerical analysis we have calculated the nearby value for power density which is  $1408 \text{ W/m}^2$ . Figure 15 shows the comparative results of power density value for same temperature range 600k and current density parameter.

**Comparison results for power density**

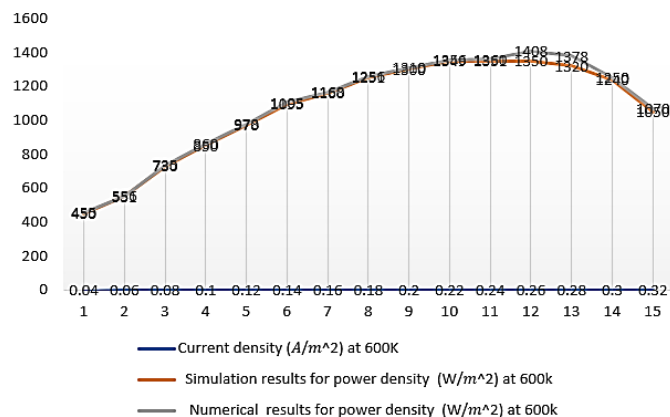


Figure 15. effect of power density for temperature range

**F). experimental result**

The result for current density vs power density and for cell voltage vs current density which we have calculated by numerical analysis, now we compared the same results with experimental results for validation. Figure 16 shows the result for current density vs cell voltage, for both cases it shows that as cell voltage decreases , current density increases. While Figure 17 shows that result for current density vs power density , for both cases it shows that as current density increases , power density also increases as current density is a function of power density.

**Current density i vs  $V_{cell}$**

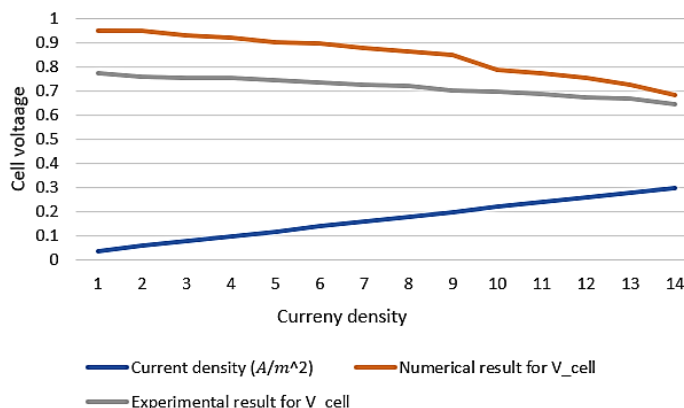


Figure 16. comparative results for effect of current density on cell voltage



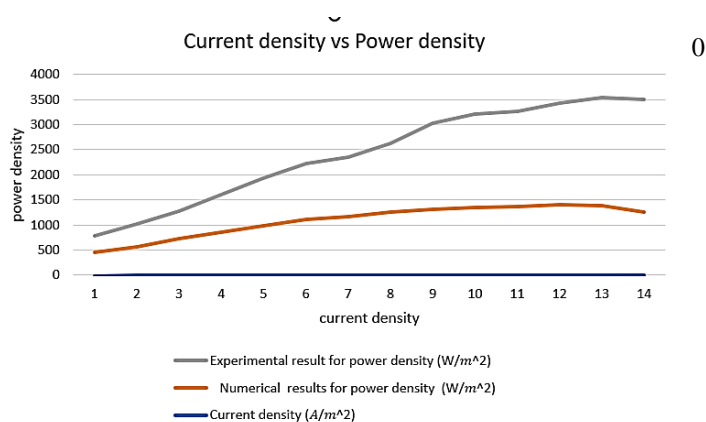


Figure 16 . comparative results for effect of current density on power density

## Conclusion

By studying & Comparing the result for power density and polarization curve for temperature variation 800k, 700k, 600k. We Conclude that when we decrease the operating temperature range from 800k to 600k, all the Polarization losses like ( Activation losses, ohmic losses & concentration losses ) which are present at the interface layer between anode and electrolyte gets decreases. According to the given cell voltage equation ( $V_{cell} = E - \eta_{act} - \eta_{ohmic} - \eta_{conc}$ )

We can also observe the when we decrease the polarization losses, the overall value for cell voltage get maximum. Therefore the value for Current density & power density will get increases. Hence, at temperature 600k as all losses gets reduced & we have achieved maximum power value which is  $1351 \text{ W/m}^2$  for an unit cell. Further for validation of our study, we have compared the simulation results with numerical results. In numerical analysis we have achieved value  $1408 \text{ W/m}^2$  for power density.

## Future scope

In automobile industries fuel cell is a upcoming future technology, fuel cells can power cars using green hydrogen which replace the fuel petroleum. As it is also a powerful green energy source so it will also help in reducing gas emission and global warming effects. By using various types of carbon based nanomaterial, metal based nanomaterial like (Graphene, Ysz, CNT etc.) , it will help to enhance the performance of fuel cell, reduce overall weight, also help to make it compact in size and it helps to reduce the pollution and globalwarming

## Nomenclature

E	Youngs modulus
F	Faraday's constant: $96,487 \text{ C mol}^{-1}$ [30]
G	Shear modulus [30]
i	Current density ( $\text{A m}^{-2}$ ) [30]
io	Exchange current ( $\text{A m}^{-2}$ ) [30]
$\square$	Permeability of porous electrode ( $\text{m}^2$ ) [30]
K	Bulk modulus (pa) [30]
P	Pressure (pa) [30]
Po	The reference pressure (pa) [30]
R	Univernal gas constant [30] ( $\text{J mol}^{-1} \text{ k}^{-1}$ )
To	Cell temperature (k)
v	Poission ratio
$\alpha$	Charge transfer coefficient
$\varphi$	Porosity
$\phi$	Potetinal (v)
t	Electrolyte thickness
$\eta_{act}$	Activation Polarization
$\eta_{ohmic}$	Ohmic Polarization
$\eta_{conc}$	Concentration Polarization
Vcell	Cell voltage
Vpol	Polarization voltage
Eo	Nernst voltage
Pd	Power density ( $\text{W/m}^2$ )

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