The Ohmic and activation over-potential in Anode-Supported Solid Oxide Fuel Cells

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Abstract— **A multi-dimensional model has been established to investigate the performance of anode-supported SOFC fuel cell with two different configuration, :i) the Anode Supported Planar Solid Oxide Fuel Cell (ASP_SOFC) with channel gas surface 1mm² and ii) ASP_SOFC with channel gas surface 0.25mm². The numerical simulation was realized with a SOFC fuel cell model based on the ANSYS FLUENT computational fluid dynamics (CFD) software. The simulation results were illustrated polarization curves including J–V,J–P, Ohmic and activation over-potential curves. It was found that the increase in channel surface has more significant influences on the cell performance. The model is validated using one of the available numerical results from previous researches the comparison between the numerical model and the reported results shows very good agreement.**

Keywords— Performance Solid oxide fuel cell, ANSYS FLUENT, Ohmic over-potential, activation over-potential.

I. INTRODUCTION

Fuel cell technology, a core component in a hydrogen-based energy economy, has the advantages of high energy conversion efficiency, low pollution, and no dependency on depleting fossil resources. Significant progress has been made in the state-of-the-art in materials, design, and fabrication; however, the widespread commercialization of most fuel cells is still limited by issues such as high cost and low durability [1,2]. Mathematical models are effective tools in understanding and optimization of various transport and electrochemical processes, leading to cost reduction and improved performance and durability.

The Solid Oxide Fuel Cell (SOFC) is an all solid type of high-temperature (600-1000°C) fuel cell that can directly convert any mixture of hydrogen, carbon monoxide and methane into electricity. Solid-oxide fuel cells (SOFCs) have the highest performance and durability. [3]

II. SOFC OPERATING PRINCIPALE

SOFC fuel cell composed of a fuel-flow channel, anode gas diffusion layer, anode catalyst layer, electrolyte, cathode catalyst layer, cathode gas diffusion layer, air-flow channel, and anode and cathode collectors [4].The schematic view of SOFC is depicted in Fig. 1. For an SOFC cell, water is formed at the anode. Electrochemical reactions at the anode and cathode respectively [5]:

At Anode : $H_2 + O^{2-} \rightarrow H_2O + 2\ e^-$

At Cathode : $\frac{1}{2}O_2 + 2\ e^- \rightarrow O^{2-}$

The overall cell reaction is $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

The cell voltage is the operating voltage of the cell, resulting from the collected differences in the electric voltage between the various phases in the cell [6]. The operating cell voltage depends on the polarizations losses and can determined by Nernst equation, as follows:

$$V_{cell} = E_{Nernest} - \eta_{Ohm} - \eta_{act} - \eta_{con} \qquad (1)$$

The voltage evaluation is carried out based on the knowledge of the cell voltage from the Nernst equation [6-8].

$$E_{Nernest} = -\frac{\Delta G}{2F} + \frac{RT}{2F}\ ln\left(\frac{P_{H_2}.P_{O_2}^{0.5}}{P_{H_2O}}\right) \qquad (2)$$

Where p (Pa) terms are the partial pressures of reacting species, R (J mol^{-1} K^{-1}) is the universal gas constant, T (K) the temperature and F (C mol^{-1}) the Faraday's constant. ΔG(J mol^{-1}) is the change of Gibbs free energy.

$$\eta_{Ohm} = \sum R_{Ohm}\, j \qquad (3)$$

$$\eta_{Act} = \frac{RT}{n\alpha F} ln\left(\frac{j}{j_0}\right) \qquad (4)$$

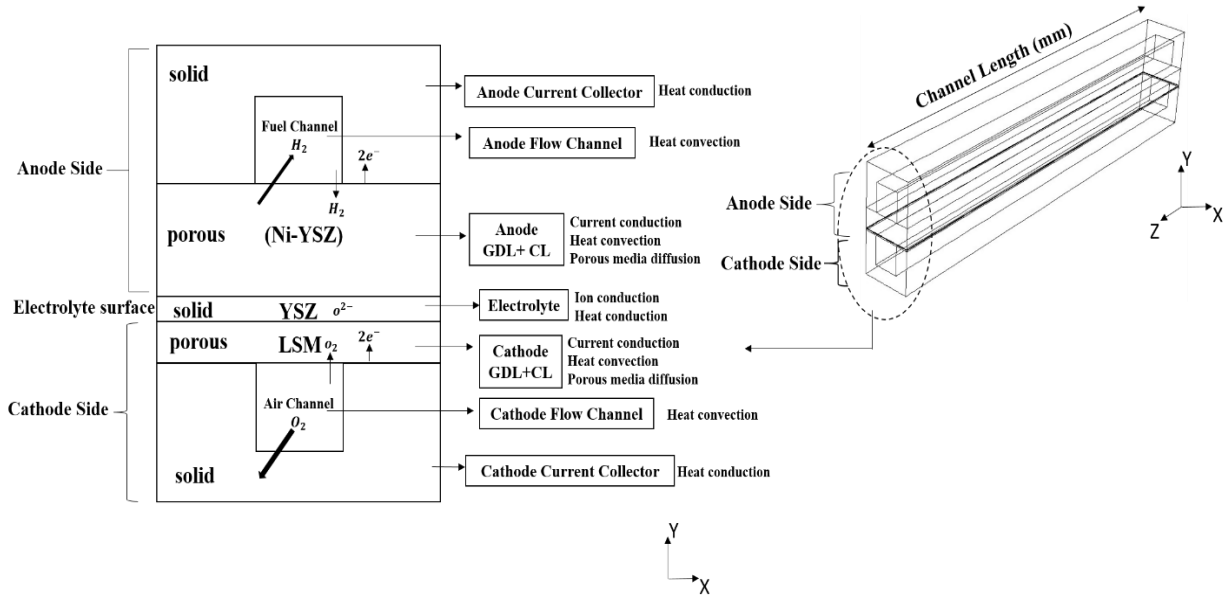

Fig. 1: 3D view for a planar SOFC counter-flow

$$\eta_{Con} = \frac{RT}{nF} ln\left(1 - \frac{j}{j_0}\right) \quad (5)$$

Where η_{Ohm}, η_{act} and η_{con}, are the Ohmic, activation and concentration losses over-potential respectively.

The details of individual over-potential above can be obtained from Ref [9].

Mathematical models of SOFC were derived from coupled partial differential equations describing the transport of charges, mass, momentum and energy. Additionally, knowledge of Bolter-Volmer equation were essential for the development of the model. In this study, the SOFC is simulated through solving its three dimensional, and steady-state governing equations via finite volume approach by using ANSYS Fluent 18.1 software.

The applicable equations are:

- Mass conservation equation [10]:

The steady state mass conservation equation is defined as:

$$\nabla.(\varepsilon\rho v) = S_m \quad (6)$$

Where ε is the porosity, ρ (kg m^{-3}) the density of gas mixture, v (m s^{-1}) the velocity, and S_m (kg m^{-3} s^{-1}) the mass source term.

The source terms of each conservation equation are discussed in detail by Ref [10-14]

- Momentum equation [10]:

Considering the steady-state momentum conservation equation at low Reynolds number:

$$\nabla.(\varepsilon\rho vv) = -\varepsilon\nabla p + \nabla.[\varepsilon\mu(\nabla v + (\nabla v)^T)] + \frac{\mu\varepsilon^2}{k_g} v \quad (7)$$

Where k_g gas phase permeability (m²), and μ (kg m^{-1} s^{-1}) the dynamic viscosity.

- Species conservation [10]:

$$\nabla.\left(-\rho y_i \sum_{j\neq i}^{n} D_{eff,ij} \nabla x_j + \rho v y_i\right) = S_i \quad (8)$$

Where y_i is the mass fraction of specie i, D_{eff} (m² s^{-1}) the effective diffusivity coefficient between specie i and j, x_j the mole fraction for specie j, and S_i (Kg m^{-3} s^{-1}) the source term for specie i.

- Energy equation [10]:

Steady-state energy conservation equation has the following form

$$\nabla.\left(\varepsilon p c_p v T\right) = \nabla.\left(k_{eff}\nabla T\right) + S_T \quad (9)$$

Where c_p (KJ Kg^{-1} K^{-1}) is the specific heat capacity, k_{eff} (W m^{-1} K^{-1}) the coefficient of thermal conductivity, and S_T (W m^{-3}) the heat source term.

- Charge transport [15,16]:

The charge conservation equation is solved for the involved charge transport in the ionic/electronic phase. Which are allowed in the anode and cathode electrodes, however in the electrolyte only ionic transport is allowed. It is assumed that the electronic transport is only allowed for current collector so charge balance can be described according to Ohm's law:

Electronic charge Balance

Anode electrode layer

$$\nabla.(\sigma_a \nabla \emptyset_{el}) = -J_a A_V \quad (10)$$

Cathode electrode layer

$$\nabla.(\sigma_c \nabla \emptyset_{el}) = -J_c A_V \quad (11)$$

Ionic charge balance:

Electrolyte layer

$$\nabla.(\sigma_{ele} \nabla \emptyset_{i0}) = 0 \quad (12)$$

Anode electrode layer

$$\nabla.(\sigma_a \nabla \emptyset_{i0}) = J_a A_V \quad (13)$$

Cathode electrode layer

$$\nabla.(\sigma_c \nabla \emptyset_{i0}) = J_c A_V \quad (14)$$

Where: σ_a and $\sigma_c$is the electrical conductivity for both anode and cathode and J_a and J_c shown in (15) and (16) are the volumetric current densities of anode and cathode. Based on the general Butler-Volmer equation [10], can be calculated as follows:

$$J_a = j_{0,a} A_V \left(exp\left(\alpha \frac{2F\eta_{act,a}}{RT}\right) - exp\left(-(1-\alpha)\frac{2F\eta_{act,a}}{RT}\right)\right) \quad (15)$$

$$J_c = j_{0,c} A_V \left(exp\left(\beta \frac{4F\eta_{act,c}}{RT}\right) - exp\left(-(1-\beta)\frac{4F\eta_{act,c}}{RT}\right)\right) \quad (16)$$

Where $j_{0,a}$ and $j_{0,c}$ (A m^{-2}) are the reference exchange current densities of anode and cathode as described in detail by Ref [17]. A_V (m^2 m^{-3}) is the reactive surface area per unit volume.

III. MODEL DESCRIPTION

A geometric modeling and meshing software GAMBIT (version 2.4.6) was used for developing the model. The design is a counter-flow SOFC with anode supported Details of the dimension are show in are shown in TABLE 1. Different cell models are considered, depending on the surface channel dimension.Fig.2 demonstrates the schematic of SOFC which it takes in our study consisting of the gas channels, gas diffusion layers (GDL), electrolyte, catalyst layers (CL) and current collectors.

Appropriate mesh generation directly affects the results of the simulation results and the time for simulation. In addition, the study independency mesh another important step that has to be verified for numerical analysis, and to ensure that the model results are independent of the grid size. GAMBIT software (version 2.4.6) is used for mesh generation in this study. The domain was divided into hexahedral volume elements in Gambit. The whole computational domain contains 270.000 cells mesh is found to provide a sufficient resolution in the first based reference model. The results are shown in Fig. 3.

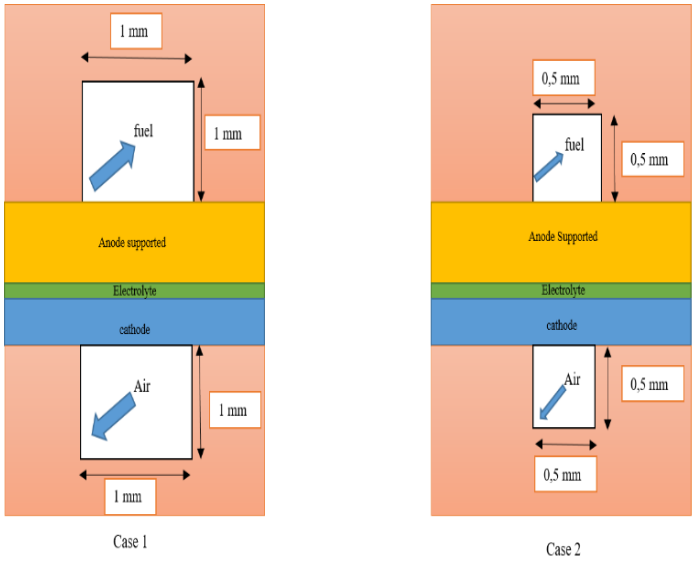

Fig. 2: Dimension gas channel cases studies.

A. *Boundary condition*

In this study, the "mass flow inlet" and "pressure outlet" boundary conditions were assigned at the inlet and outlet ports of the anode and cathode gas channels, respectively. The "wall" boundary condition are considered as adiabatic was assigned at the terminal surfaces of current collector (anode and cathode) and Cell surroundings. Details of the boundary condition are show in TABLE 2.

The fuel is fed into the fuel cell as a mixture of gases. The gas mixture that is fed through the anode inlet consists of hydrogen and water vapor. The gas that is fed through the cathode inlet consists of oxygen. The mass fraction for hydrogen is set as 0.97 and the mass fraction for water vapor in the anode fuel mixture is set as 0.03. The mass fraction for oxygen is set as 1 at the cathode side.

Steady-state simulations and second order discretization for all equations were used in this study Multigrid cycle was changed for F-Cycle for all equations. Stabilization method was chosen (Bi-conjugate gradient stabilization) BCGSTAB for species concentrations, water saturation, electric and protonic potential. Terminal restrictions were changed 0.001 for species concentrations, water saturation and for 0.0001 for electric and protonic potential. Maximum number of cycles was increased for 50. [18]

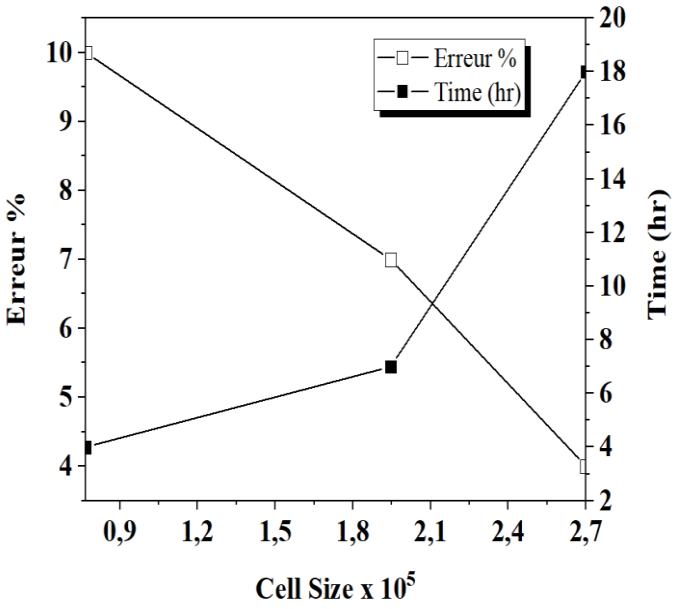

Fig. 3 : Mesh Independency analysis.

B. *ANSYS simulation*

There are many studies in the literature that have utilized the ANSYS SOFC module for modeling the simulations. CFD code is used to solve the model equations for planar SOFC with different surface channel. After create geometry and mesh, the next step that should be taken is reading the mesh file with the solver. The SOFC model is checked for its dimensions in ANSYS Fluent 18.1 and then it is checked for the quality and ensured no negative volume exists. The SOFC Fuel cells model is activated in Fluent from the add-on module and the open-circuit voltage is set to 1.05 V. Both the anode and cathode zones in the model are defined appropriately to the zones available in the mesh. Except the current collectors, all the parts in the fuel cell are defined as fluid zone, while the current collectors in the anode and cathode side are defined as solid in the cell zone condition. After setting up the boundary conditions, and solution control parameters, initialize the solution and run calculation. The output results from this 3D model include local current density, species and temperature distributions on the sinusoidal and single planar SOFC.

Table 1- Geometrical Parameters

zone	*Dimension(mm)*
Cell width	2
Cell length	19
Anode thickness	0.700
Cathode thickness	0.05
Electrolyte thickness	0.01
Channel height	Validation and Case 1: 1 Case 2: 0.5
Channel width	Validation and Case 1: 1 Case 2: 0.5
Current collector height	1.5

C. *Model validation*

The cell voltage versus as the current density curve for the presented model was compared with data [19]; this comparison is shown in Fig. 4, showed a good agreement.

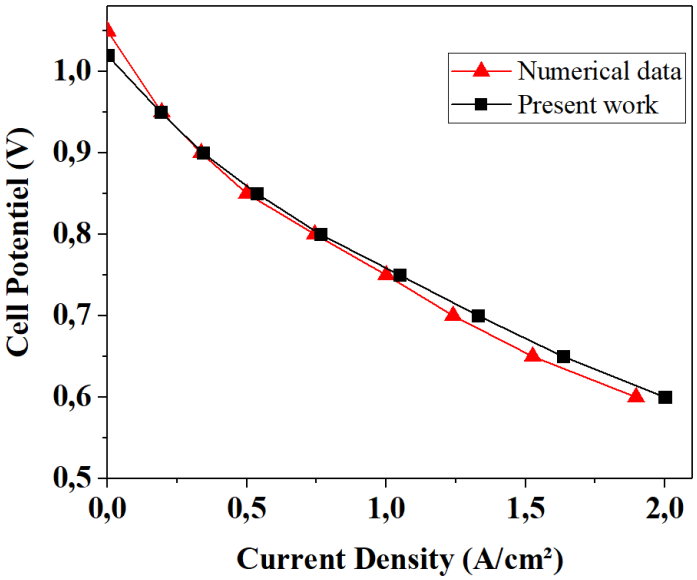

Fig. 4: Comparison between our results and numerically data obtained by [19].

Table 2- Boundary Condition		
parameter	***BC***	***Temperature***
Hydrogen inlet	Mass flow inlet (kg/s) 1.141×10^{-8}	1123 K
Oxygen inlet	Mass flow inlet (kg/s) 2.287×10^{-7}	1123 K
Hydrogen outlet	Pressure outlet	Convection
Oxygen outlet	Pressure outlet	Convection
Terminal anode collector	Wall	Adiabatic
Terminal cathode collector	Wall	Adiabatic
Cell surroundings	Wall	Adiabatic

IV. Result

The results are shows and compared between two cases and discussed in detail.

A. Performance Study

Polarization curves are generally used to describe the characteristics of a fuel cell and to understand the phenomena of electrochemical reactions; Fig. 5 shows the predicted cell voltage and power density as a function of current density, in case 1 and case 2, for the previous conditions operating. The performance of a cell is significantly highest in case 1 than case 2. The maximum power density is 2.03 W/cm² at 5.08 A/cm² while the case 2 the maximum power density is 1.06 W/cm² at 2.65 A/cm².Fig. 6, it was found that there seems to be little difference between case 1 and 2, for Ohmic over-potential. This can explain by the small dimensions of the cell leads to reduce the surface of reaction. In fact, it was true that. Because according (3), it was found Ohmic over-potential is proportional with current density. On the contrary the activation over-potential it was found to decrease with increasing surface channel as shows in Fig.7**.** Finally, it can conclude that the effect on performance is caused by losses and this is explained by the (1).

Table 3-Maximum rate of hydrogen consumed in anode. (%)	
Case 1	0.68
Case 2	0.49

Table 4-Maximum produced rate of steam water in anode/electrolyte interface. (%)	
Case 1	0.672
Case 2	0.585

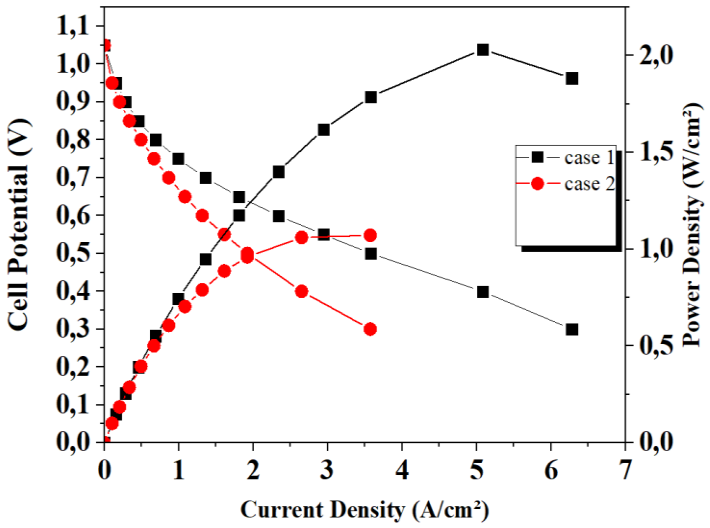

Fig. 5: Polarization curves in cases 1 and 2.

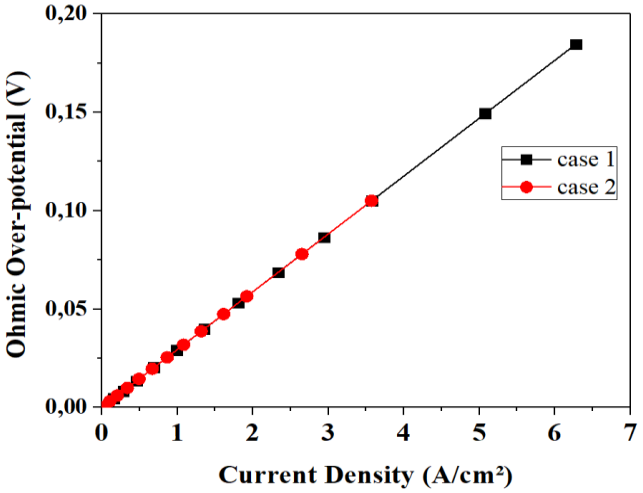

Fig. 6: Ohmic over-potentials curves in cases 1 and 2.

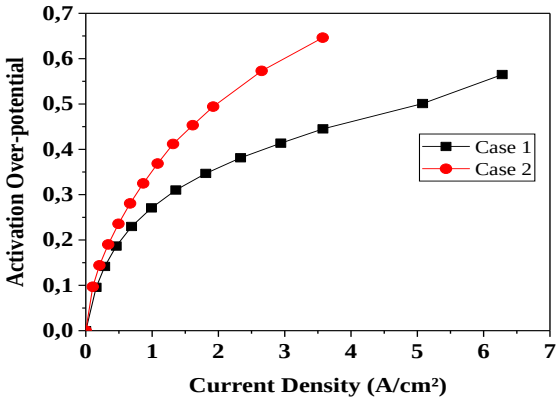

Fig. 7: Activation over-potentials curves in cases 1 and 2

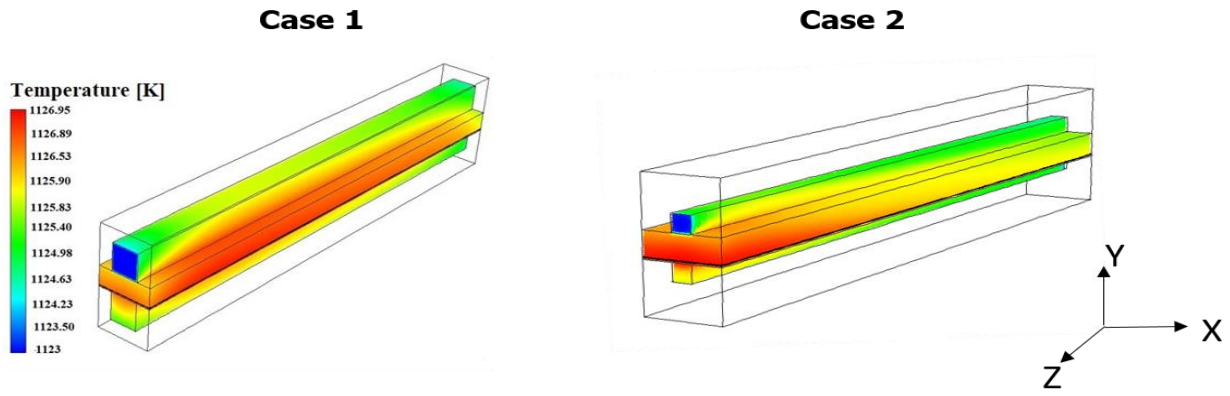

Fig. 8: distribution of temperature in cases 1 and 2, at 0.6 v.

B. Distribution of temperature

An increase in temperature values is clearly remarkable from the inlet to the outlet of the cells for both cases as shows in Fig. 8. The case 1 led to higher temperature values as compared to the case 2. The maximum temperature value is located in the electrolyte is 1126.95 K and 1125.85 K for case 1 and case 2 respectively. That due to the higher surface led to accelerate the kinetic of reaction, thus resulting in it an increase in rate of reaction as reported in literature [20,21].

C. Mass fraction species

The hydrogen mass transfer is from the anode channel to the interface with electrolyte. Fig. 9 shows the variation of the species mass fraction along the z-direction at different surface channel. Based on the figure, the hydrogen mass fraction decreases along the anode flow direction due to hydrogen is consumed by the electrochemical reaction. On the other hand, decreasing hydrogen mass fraction increase water mass fraction from inlet to outlet. Better distribution resulting a better value for utilization Fuel U_{fuel}. Furthermore, increasing surface channel leads to a significant increase of hydrogen consumption and increase of water produced as shown in tables 3 and 4 respectively. The highest hydrogen consumption are 0.68 and 0.49 for case 1 and 2 respectively. The highest water produced are 0.672 and 0.585 for case 1 and 2 respectively.

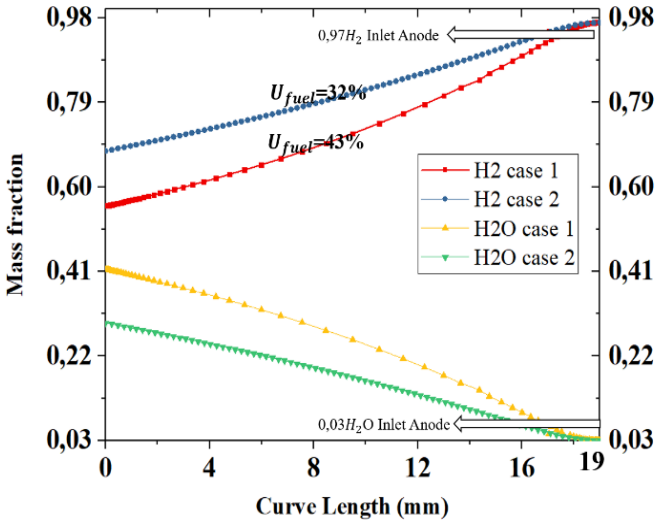

Fig. 9: Variation of H_2 and H_2O mass fraction distribution along the anode channel in cases 1 and 2, at 0.6

V. CONCLUSION

The performance of a SOFC fuel cell is investigated numerically by changing the geometry of the channels surface. A complete three-dimensional model for SOFC fuel cells has been used and a series of tests are carried out to investigate and validate the numerical results of the polarization curve under the normal conditions. In addition, a step-by-step procedure for using SOFC module was presented, providing readers with a deep insight into the software. Geometry, meshing size, all boundary condition, solution method, flow zone types, and solver settings were precisely discussed. SOFC fuel cell model 3D shown that is capable of solving mass, momentum, energy, electric potential, and species equations properly. Furthermore, the results show that a high performance was observed by using high surface for the channels of anode and cathode sides. Also the results show that the effect of temperature on the performance of the cell is so important that by increasing the surface channel the cell performance enhances that it is due to the decreasing of activation over potential and increase in the electrochemical reaction. Which hurts the latter to increase Ohmic over potential. On the other hand, the effect of the surface channel on the hydrogen mass fraction consumption is more important as discussed earlier. Similarly, the water produced at the interface anode/electrolyte are high when the surface channel is high.

NOMENCLATURES

A_V	reactive surface area per unit volume, m^2m^{-3}
c_v	specific heat capacity, kJ kg^{-1} K^{-1}
D	gas diffusivity, m^2 s^{-1}
$E_{Nernest}$	Nernst potential, V
F	faraday's constant, C mol^{-1}
J	exchange current density, A m^{-3}
j	current density,A m^{-2}
ΔG	Gibbs free energy change,J mol^{-1} K^{-1}
k_a	gas phase permeability,m^2
p	gas pressure, Pa
R	universal gas constant, J mol^{-1} K^{-1}
s	source term,Kg m^{-3} s^{-1} ,W m^{-3}
T	temperature, K
U_{fuel}	Factor utilzition fuel
V_{cell}	cell potential, V
x	mole fraction
y	mass fraction

Greek Letters

0	standard state
α	transfer coefficient in anode
β	transfer coefficient in cathode
ε	porosity
Ø	Exchange potential (V)
η	overpotential, V
k	coefficient of thermal conductivity,W m^{-1} K^{-1}
σ	specific conductivity, s m^{-1}
μ	fluid viscosity, Kg m^{-1} s^{-1}
v	velocity, m s^{-1}
ρ	Density, kg m^{-3}

Subscripts and Superscripts

a	anode
act	activation
c	cathode
$conc$	concetration
eff	effective
el	electronic
ele	electrolyte
j	species j
i	species i
$i0$	ionic
LSM	cathode material
Ni-YSZ	anode material
ohm	ohmic
SOFC	solid oxide fuel cell
YSZ	electrolyte material

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