

## Simulation of Flow Field Pattern Influence on the Hydrogen Consumption in A PEMFC

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**Abstract:** Simulations results are presented in this paper, which were obtained on investigating the effects of flow patterns on the hydrogen consumption in a proton exchange membrane fuel cell (PEMFC). In this study, a 3-D computational model was developed to investigate the influence of the flow and depth of the channels on hydrogen consumption. Simulation results showed the influence of depth in the distribution of hydrogen concentration. The flow channel pattern adopted in this study is the serpentine flow channel.

*Keywords:* fuel cell, bipolar plate, simulation, flow field

### 1. INTRODUCTION

In recent years, there has been great interest in industry and science to study alternative energy generation with varied levels of success. Some of them are; wind turbines, small-scale hydroelectric plants, biomass generation systems, micro turbines, photovoltaic arrays and fuel cells etc. The latter ones represent a promising alternative for power supply. Recent technical analysis and economic developments have made fuel cells to be considered as an environmentally friendly technology, with an operating system virtually free of noise and high efficiency [1]. An important feature in the planning of power generation based on fuel cells is, in fact the effect on stability of the system. One important element in these systems is the proton exchange membrane, which has been assigned an important relationship on the efficiency of the fuel cell.

Important advances have been made in the improvement of the proton exchange membrane, principally in raising performance and durability, reducing the cost of energy production. Also, there has been encouraging understanding in the basic aspects of the components of the cell and all aspects of design and performance optimization. For example, degradation of membrane associated mainly with the reaction of the species, has encouraged several research groups develop chemical methods to improve the material performance and reduce the conditions that accelerate the degradation of the membranes. Other factors are related to poor water

management and the development of new catalysts for the fuel cells.

Variations in the operating flow pressure in a fuel cell is affected by even small variations of the permeability values of the diffusion layer. Hence, it is important to consider the transport phenomena at the interior of the cell. So also its performance and physical properties of its components. For example, different values in the permeability of the gas diffusion layers and the gas flow can generate variations in the operating pressure [2,3].

Several researchers have oriented their efforts to develop important tools for modeling and simulation of components of fuel cell, with the purpose of optimizing the design parameters and manufacturing processes against mechanical failure and chemical degradation of materials. Existing models are structured to solve problems in three-dimensional conservation equations, with heat transfer and electrochemical reactions [4-7].

A lot of commercial software have been developed and used to model fuel cells. The commercial softwares are a good alternative, such as virtual laboratory because they allow the user to have a set of tools to build and model subroutines for certain specific processes. However, it is necessary to establish models that include the influence and characteristics of the flow dynamics and its interaction with the porous media (diffuser, catalyst layer, membrane), and the influence in operating conditions in a temporary state. Most of the information about fuel cells is concerning the material used for fabricating the cell, the chemical processes involved and the applications that can be given to these cells [8-13].

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A fuel cell is a device that consists of two regions defined as anode and cathode. Between the cathode and the anode there are the membrane and catalyst layers. Hydrogen flows into the anode and is dissociated into protons and electrons. The protons are transported through the membrane to the region of the cathode, while electrons flow through an external circuit to generate electricity. Finally, the protons and electrons combine in the region of cathode with oxygen to produce water [14].

The mathematical modeling of a fuel cell can be achieved by solving the 3 dimensional conservation equations for mass, momentum and energy and the equation that contemplates the associated chemical reactions. Furthermore, from the viewpoint of chemical or physical processes that could occur in a fuel cell there have been proposed sub-models. The use these sub-models are important to differentiate between types of analysis done from one cell to another, because the results can be very different. Currently, there exist a large number of fuel cell models, but only a few describing the operation of the fuel cell, this is due to the complexity and the relationship among the processes that take place inside the fuel cell at macro and microscopic level. Therefore the use of models or sub-models oriented to a specific solution may be helpful.

These models do not permit the most detailed understanding of chemical and electrochemical processes, electrical flow, heat generation etc. in a fuel cell simultaneously. This is due to existing computational limitations. This urges the necessity to continue exploring and implementing models whose methodology allows a detailed understanding of the electrochemical processes and their interaction with the dynamic changes taking place during the operation of a fuel cell.

## 2. THE THREE-DIMENSIONAL MODEL

### 2.1. Model Description and Assumptions

In this paper, the computational model contemplates the flow channel region of the bipolar plate with a serpentine type configuration, which simulates the distribution of  $H_2$  gas across the electrode surface. A second region is the diffusion layer, where the gas is transported or transferred via diffusion and convective transport through a porous medium. A third region is the catalytic layer where it occurs dissociation of hydrogen molecules into hydrogen ions and electrons. This study was conducted to determine the influence of geometry on flow dynamics and the distribution of the concentration of  $H_2$  in a fuel cell model.

Figure 1 shows schematically the three regions considered in the model. The active area, that is to say the area of the electrode surface in the computational domain, is 40 mm long and 40 mm wide.

### 2.2. The Model Considerations

The following assumptions were done in the computational model

1. Steady State
2. Effect of gravity on the system is negligible
3. Isothermal system
4. Laminar flow
5. The permeability of the catalytic layer is equal to the diffusion layer
6. The formation of liquid water is not considered
7. Compressible ideal gas flow

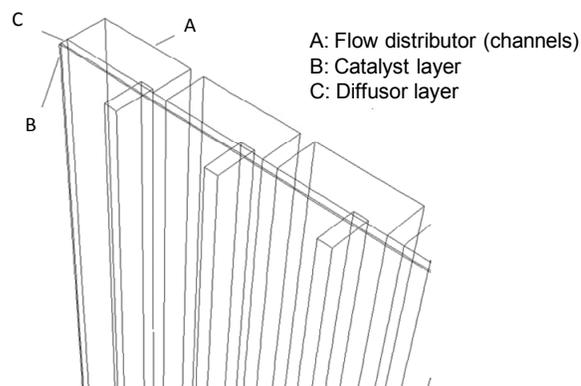


Figure 1. The geometrical model

### 2.3. The Governing Equations

In this model we considered the conservation equations of mass, momentum and energy for the area of geometric domain. Additionally we contemplated a term due to the electrochemical reaction in the domain of the catalyst layer corresponding to the dissociation of hydrogen in the domain. For this we integrated the available functions in the program Fluent for the model.

### 2.4. The reaction

The breaking of a chemical bond requires energy, inversely when a bond is formed energy is released. In the early stages of a chemical reaction the energy released during formation of the chemical bond is not enough to break the bond again. It needs extra energy, which is considered to be coming from the kinetic energy of the molecules [3]. Thus, the molecules must collide with enough force to provide this extra energy. Only a small fraction of all collisions have sufficient kinetic energy so that the reaction takes place, hence the speed of reaction is low.

The hydrogen evolution reaction is performed in the same way and it is very important in the functioning of fuel cells based on  $H_2$ . Therefore, it is important to understand the chemical and electronic states of the species absorbed on the surface of the electrocatalyst, as this largely determines the efficiency of a fuel cell. The catalytic layer has two functions. First, it provides the surface where the hydrogen molecules are dissociated and second, it serves as an electrical conductor for the external circuit. These characteristics that define the catalytic active sites where the decomposition of  $H_2$  is carried out as follows:



Where, A is defined as the active site.

Since  $H_2$  is a gaseous substance it is defined as the substance that is trapped in a solid (porous medium of the fuel cell). Thus, the monatomic hydrogen originates from the gas phase and prevents the dissemination of the same to the diffusion layer and the distribution channel of the bipolar plate. On the other hand, the active sites identified as A, have no reaction with the gas phase and only appear as an inert body, which can absorb the energy released in the reaction [4].

The reaction mechanism considers that the systems (fuel cells)

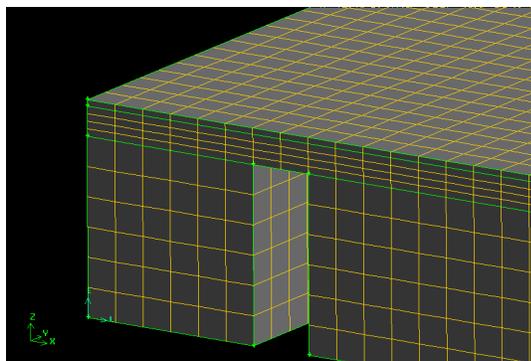


Figure 2. Detail of the mesh

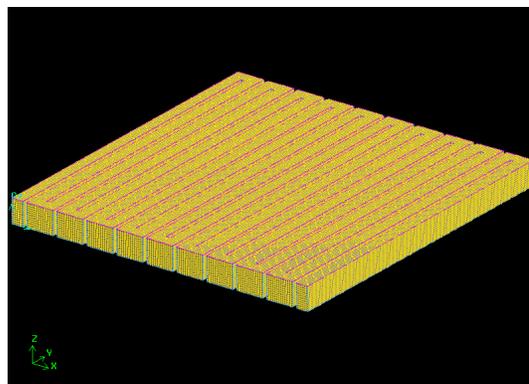


Figure 3. Details of the full mesh

rarely operate with 100% pure substance. A hydrogen fuel cell is humidified to keep the humidity of the membrane. The system considers an isothermal type process, open flow with a pure substance with variations in pressure and therefore density and concentration are minimum. Likewise, the Fluent software can solve n-1 equations of transport of chemicals for a chemical system with n as the sum of all mass fractions which is always equal to 1, obviously in a system with a single substance does not resolve any transport equation [5]. The reaction rate used was described earlier, and assumes that the reaction mechanism only considers the uniform concentration of  $H_2$ . For the solution process, this equation was integrated with FLUENT to generate a program in C language.

### 2.5. The Porous Media

Both the diffusion layer and the catalytic layer are assumed as porous media, allowing the convective motion of hydrogen molecules through them. For both layers it is assumed isotropic permeability of  $1 \times 10^{-12} \text{ m}^2$ . Since the diffusion layer is a good conductive medium, this allows the transport of electrons between the collector plate and the catalytic layer. Normally this material is made of carbon paper or cloth, suitable due to its conductive properties and resistance to corrosion.

Unlike Kumar et al. [2], in this case FLUENT facilitated us with the incorporation of models for porous media including Darcy's law and the inertial resistance, which allows the definition of the boundary conditions for all porous areas and setting the values of the diffusivities. It is worth mentioning that due to the assumption of isotropy, the three corresponding diffusivities in each direction are equal.

### 2.6. The Boundary Conditions

Operating Temperature	Inlet Flow	Operating Pressure	Flow Direction
350 K	$2.5 \times 10^{-7} \text{ [kg/s]}$	2 atm.	Normal

### 2.7. Operation of the Cell

To evaluate the performance or efficiency of the cell, hydrogen consumption was calculated using a mass balance relating to flow into and out of the model system. In turn, the flows were determined from the flow report of the mass fraction of species by the software.

## 3. RESULTS AND DISCUSSION

### 3.1. Validation

To validate the model and the methodology adopted in this study, we simulated the conditions used in the work reported by Kumar et al. [2]. They conducted simulations, which were validated with experimental results. The geometrical model corresponds to a channel width of 1.5 mm, channel spacing of 0.5 mm and a depth of 1.5 mm. The thickness of the diffusion and catalytic layer were 0.25 mm and 0.05 mm respectively. The overall dimensions of the cell were 40 mm x 40 mm x 1.8 mm. Figure 2 and 3 show details of the mesh generated in the geometric model of the present study.

As a first step, the code validation was carried out by numerical determination of the global analysis of continuity, momentum and heat transfer. Also, it took into account the relative difference with respect to the numerical solution regardless of the mesh. Finally, the results presented are based on the mesh dependence criterion analyzed.

The hydrogen consumption was calculated as 82.6% compared to 84.8% reported in the literature [2], representing a 2.6% difference, which can be justified because of the difference in the methodology adopted. Having these results we proceeded to carry out the simulation of the problem as the case study, whose parameters are listed below.

Parameter	Value
Diffusion layer thickness	0.11 mm
Porosity	80 %
Catalyst layer thickness	0.012 mm
Separation between channels	0.4 mm
Distribution channels of square section	0.8 mm

Figure 4 shows the molecular hydrogen concentration ( $\text{kmol/m}^3$ ) in the cell, at the plane that divides the diffusion layer and the bipolar plate. There is a gradual decrease in concentration from the corner near the entrance towards the other parts of the channels, but since the exit is not diagonally opposite to the entrance, this distribution is distorted towards the corner near the exit. The hydrogen consumption determined in this case study was only 20.4%, which

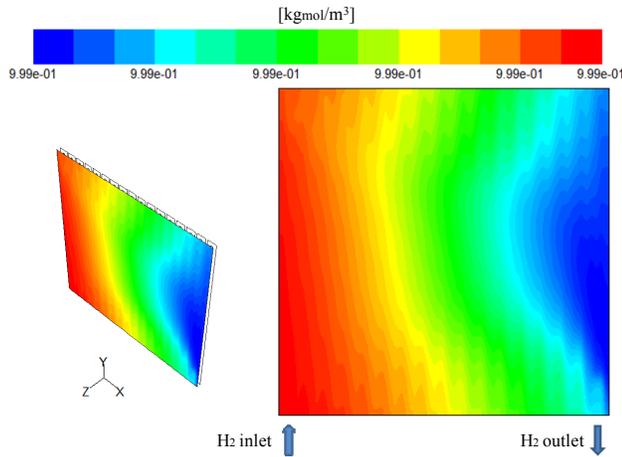


Figure 4. Molar concentration contours: case study

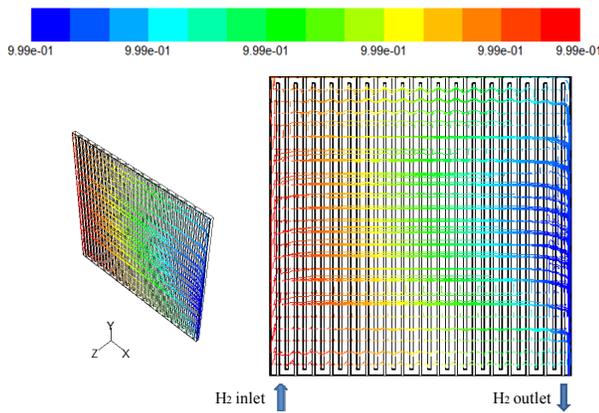


Figure 5. The flow path lines

represents low fuel utilization. This is attributed to the cell size of the case study, the thickness of the diffusion layer and the catalytic layer, with the catalytic layer thickness having the greatest influence as it relates directly to the amount of active sites to carry out the reaction and mass transport of hydrogen flow.

Figure 5 shows the trajectory of the fluid particles. It is pertinent to note that there is no defined stream channel because the gas can flow over the separation of the channels through the porous media. This cross flow with the  $H_2$  oxidation reaction generates the distribution of  $H_2$  concentration observed in Figure 4. With these flow dynamic characteristics, the design of flow distributor in a fuel cell becomes important for the transport of the fluid for distribution on the active sites of the catalytic layer. It has been found in the literature [15-18] several studies on different aspects of the flow.

Figure 6 shows the flow velocity contour plots throughout the flow distributor. It is observed in the inflow region the formation of zones of low speed fluid, which has implications on the transport of fluid to the active sites of the catalytic layer. The existence of these low velocity zones or vortex (recirculation) generates an effect of high pressure in this area, reducing the mass transfer to the catalytic layer. Likewise, the cross flow around the geometric domain is

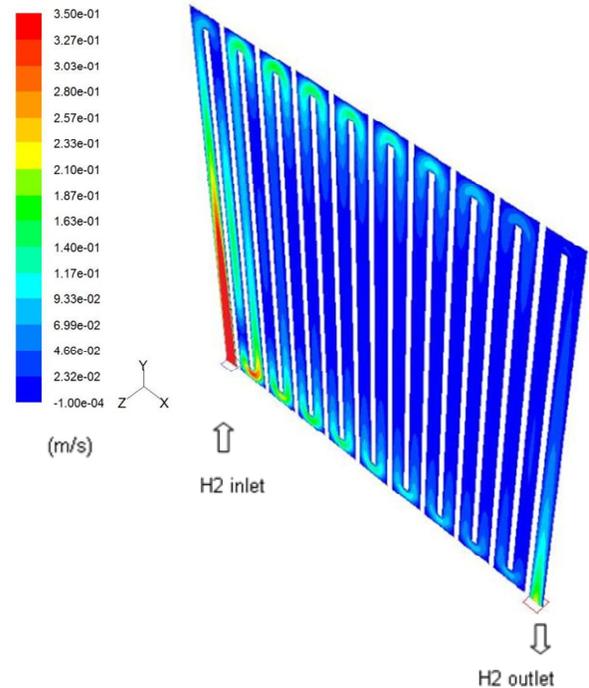


Figure 6. The velocity contours

low. This figure also highlights the influence of geometry on flow dynamics in the change of direction of the coil. Reynolds number was obtained as a function of inlet velocity of the fluid and the depth of channels. The kinematic viscosity of hydrogen at 20 °C is  $9.6 \times 10^{-5} \text{ m}^2/\text{s}$ , this value was considered as constant. Therefore, the inlet Reynolds numbers is:

$$\text{Re} = \frac{\rho HV}{\mu} = \frac{(0.0008\text{m})(0.35\text{m/s})}{(9.6 \times 10^{-5} \text{ m}^2/\text{s})} = 2.9$$

However, if we consider the average velocity until half the length of the channel from the entrance, we will have the Reynolds number as:

$$\text{Re} = \frac{\rho HV}{\mu} = \frac{(0.0008\text{m})(0.233\text{m/s})}{(9.6 \times 10^{-5} \text{ m}^2/\text{s})} = 1.9$$

These low Reynolds numbers imply a laminar flow in the channels of bipolar plate in the geometric model.

Figure 7 shows the variation of flow velocity across the coil. It is noted that the level of speed in the curve showing the recirculating flow region is in blue, which is characterized by a low convective mass transport to the porous zone, accompanied by areas of increased pressure, which reduces the efficiency of the cell. The effect of recirculation zones within the flow channels is strongly determined by the size of channels and the processes of diffusion and convection to the porous media affecting the main flow in the channel.

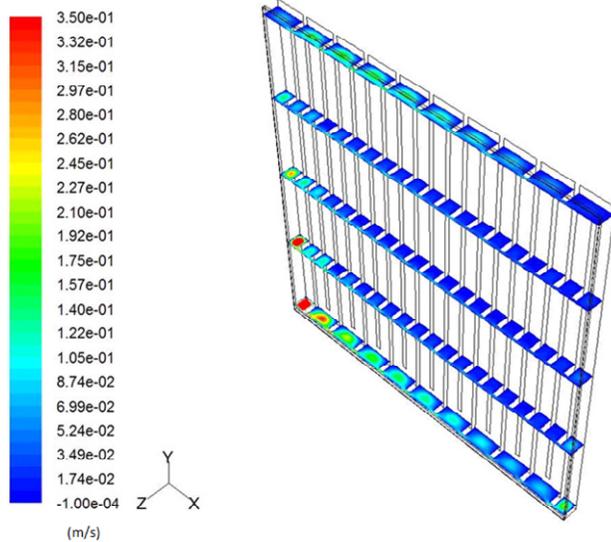


Figure 7. Isometric planes of the velocity field

#### 4. CONCLUSIONS

The results presented in this study establish a link between the convective flow through the porous boundary and the flow through the channels. The pressure drop near the exit region of the serpentine coil causes the exchange flow via diffusion is delayed, resulting in less efficiency in the dissociation of  $H_2$ . This could affect the evacuation of product water in the cathode side. The model does not predict the degradation of Pt. The hydrogen consumption according to the model validation was around 82.6%, however by reducing about 50% the cross section of the flow channels the  $H_2$  consumption was reduced to a value of 20.4%. However, authors like Dewan et al. [16] have suggested that channels of rectangular form have better current density distributions but not uniform compared to the other geometries. The reduction in spacing between channels improves the system performance, in the sense that it increases the active area in the model. Despite this, we must consider the speed regimes combined with the geometric dimensions to establish optimal levels of efficiency for the fuel cell. The Velocity field and the axial velocity of  $H_2$  are reduced as it penetrates to the interior regions of the channels. This may be attributed to the ability of the porous media to capture the  $H_2$  molecules via convective flow through porous media, increasing its dissociation in the catalyst layer. The output buffer has an effect, which reduces the convective force, reducing the effect of flooding in the diffusion layer. As a result, performance of the fuel cell is adversely affected.

#### 5. ACKNOWLEDGMENTS

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