COMSOL Modelling and Simulation of PEM Fuel Cell’s Flow Channels

Eric Robalinho¹, Edgar F Cunha¹, Alexandre B Andrade¹, Martha L M Bejarano¹, Marcelo Linardi¹, Efraim Cekinski²

¹ Instituto de Pesquisas Energéticas e Nucleares (IPEN / CNEN - SP)
Av. Professor Lineu Prestes 2242
05508-000 São Paulo, SP
eric@ipen.br
efcunha@ipen.br
abodart@ipen.br
mmora@ipen.br
mlinardi@ipen.br

² Instituto de Pesquisas Tecnológicas (IPT - SP)
Av. Prof. Almeida Prado, 532
05508-901 São Paulo, SP
cekinski@ipt.br

Abstract: Fuel cells are one of the most important devices to obtain electrical energy from hydrogen. The Computational Fluid Dynamic (CFD) is a very useful tool to explore the connection between the transport of reactants and products within the fuel cell and overall cell performance. CFD simulates hydrogen and oxygen gases flow channels to reduce the costs of bipolar plates’ production through optimization of the mass transport. In this work, two configurations of gas flow channels were studied by simulation with COMSOL software and a preliminary experimental test to verify the model applied in these configurations was performed. Two single Proton Exchange Membrane Fuel Cells – PEMFC – with 144 cm² of active area were manufactured. The first one (1) was a commercial graphite plate supplied by ELECTROCELL. The other one (2) was projected and constructed at IPEN. The serpentine flow field was chosen. The dimensions of flow field of prototype 1 were: 2 mm width and 2 mm depth channels and 2 mm ribs. In this case each part of the serpentine flow field was composed by 6 channels and 5 ribs. The dimensions of flow field of prototype 2 were: 1.5 mm width and 1.5 depth channels and 0.5 mm ribs. For this prototype, each part of serpentine flow field was composed by 12 channels and 11 ribs. A mesh study was performed on the 3D models to determine the minimum number of elements required to accurately solve the equations over the solution domain. Process simulations of diffusion in porous media and conduction/convection were studied. Once all of the global iterations had been completed, the experimental data were compared with modelling results. The graphite plate B exhibited better performance than the A one, that was validated by numeric methods. Such behavior was attributed to the higher channel area in contact with gas diffusion electrode which provides higher active area available for the gas reaction. Besides the area, higher gas velocities in flow fields decrease the gas stagnation points along the channels.

Keywords: Numerical model, CFD simulation, PEMFC, hydrogen technology.

1. Introduction

Fuel cells and hydrogen technology represent the most promising alternative pathway for automotive and stationary applications. The PEMFC offers low to zero emission for subWatt to MWatt power generation, meaning applications in transportation, industries and portable supplies units [1,2]. In this paper the role of computational tools was studied in order to verify some experimental results and demonstrate the better performance of PEMFC constructed from optimizations techniques.
The PEMFC is an electrochemical device and consists of two principal parts: (i) an electrolyte between two electrodes, an anode and a cathode with two diffusion layers, called Membrane Electrode Assembly (MEA) and (ii) gas flow field plates, called bipolar plates, in case of the stack. The plates have many functions in a fuel cell [3]: distribute reactant gases (hydrogen and air or oxygen) uniformly, collect and conduct electrical current and remove heat and water from the electrodes. The bipolar plates make the cell robust and give a rigid structure to support the impacts of portable and automotive applications. The cost of the bipolar plates corresponds up to 45% of the total cost and about 80% of the total weight in a stack fuel cell [4,5].

The search for reliable computational models is a challenge because it involves several transport phenomena: multi-component, multi-phase and multi-dimensional flow processes, electrochemical reactions, convective heat and mass transport in flow channels, diffusion of reactants through porous electrodes, transport of water through the membrane and transport of electrons through solid matrix.

The Computational Fluid Dynamic (CFD) is a very useful tool to simulate hydrogen and oxygen gases flow channels configurations, reducing the costs of bipolar plates’ production and optimizing mass transport [6-8].

2. Methodology

Two single cells of 144 cm² of active area were manufactured, called prototype 1 and prototype 2. The serpentine flow field was chosen for channel geometry. The configuration of flow field in the prototype 1 was: 2 mm width and 2 mm depth channels and 2 mm ribs. In this case each part of the serpentine flow field was composed by 6 channels and 5 ribs. The flow field of prototype 2 was: 1.5 mm width and 1.5 depth channels and 0.5 mm ribs. For this prototype, each part of serpentine flow field was composed of 12 channels and 11 ribs. In Figure 1 (a) and (b) the bipolar plates of prototype 1 and prototype 2 were showed, respectively. For these flow field configurations, the prototype 2 has 50% more channel area than prototype 1 (0.110 m² and 0.073 m² respectively).

The best-known membrane electrolyte material for PEM fuel cell is Nafion™ membrane by Dupont, which has high proton conductivity. Besides the membrane, the MEA is composed by two electrodes as catalytic layers, using platinum supported in carbon black as electro catalysts; and two gas diffusion layers (GDL) like carbon paper or carbon cloth. Fuel cell polarization measurements were carried out galvanostatically with the single cell at 70 °C, using oxygen and hydrogen with saturated water vapor (Millipore quality – Elix 3 model) at 85 °C, atmospheric pressure and hydrogen volumetric flux $8.33 \times 10^{-6}$ m³ s⁻¹.

Figure 1: Flow field channels from prototype 1 (a) and prototype 2 (b).
3. Numerical Models

The efforts of this work were concentrated in two goals. The first part was the analysis of four partial geometries consisting of the inlet and two channels with the porous media. Then, in the second place, two graphite plates were simulated to investigate the hydrogen flow, pressure drops and temperature distribution. Implementations of the modeling allowed the optimization the design of the plates and better understanding the fuel cell dynamics.

The Nonlinear solver for stationary analysis was set automatically by COMSOL, and the Spooles direct solver was selected for linear conditions [9]. The Spooles uses the multifrontal method and direct LU factorization of the sparse matrix $A$ when solves systems of the form $Ax=b$. There are several solver methods available at COMSOL Multiphysics, including the iterative ones that are the natural choice for problems with many degrees of freedom. However the iterative solvers are less stable than direct solvers and they do not always converge.

In Figures 2-5 the channels geometries are showed. The red region represents the gas inlet, the blue one is the distribution place and the green is the initial part of two channels. The area above the channels (0.25 mm thickness transparent rectangle) is the GDL. The triangular and the trapezoidal geometries have 1.5 mm depth. In the Figures 2-5 the x, y and z axis are showed.

In the Table 1 the different meshes and corresponding solutions time were compared. The convergence in these cases was obtained in 3 to 7 iterations and the relative tolerance at nonlinear solver was set on $1.0\times10^{-6}$. The refinement method was set on longest, with the best quality option. The mesh in each simulation is defined by the Number of Degrees of Freedom (NOF’S), the Number of Elements (NE) and the Minimum Element Quality (MEQ). As one can see at Table 1, the refinement of the mesh means much more solution time and availability of memory.

The flow distribution is described by two equations: Navier-Stokes (Eq.1.) and continuity (Eq.2.),
\[
\frac{\partial u}{\partial t} - \nabla \cdot (\eta \nabla u + (\nabla u)^T) + p(u \nabla u) + \nabla p = 0
\]  
(1)

\[
\nabla \cdot u = 0
\]  
(2)

where \( \rho \) denotes the density [kg m\(^{-3}\)], \( u \) the velocity vector [m s\(^{-1}\)], \( \eta \) the viscosity [N s m\(^{-2}\)], and \( p \) the pressure [Pa]. The density and viscosity of the modeled gases were calculated in function of the pressure and temperature using models offered for the CFD software.

The model uses normal/pressure boundary conditions for inlet and convective flux for outlet. The condition for porosity (porous media) was found in Navier-Stokes module in COMSOL, version 3.3, which was set on 1.0E-12 m\(^2\) for permeability of GDL.

The results in Table 1 and the pos-processing Figures and Graphics were obtained at Intel 5320 Quad Core XEON Workstation with 4 GB RAM.

<table>
<thead>
<tr>
<th>MESH</th>
<th>NOF'S</th>
<th>NE</th>
<th>MEQ</th>
<th>SOLUTION TIME (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>TRIANGULAR</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coarser</td>
<td>7351</td>
<td>957</td>
<td>0.2829</td>
<td>9.1</td>
</tr>
<tr>
<td>Coarse</td>
<td>10808</td>
<td>1464</td>
<td>0.2990</td>
<td>14.6</td>
</tr>
<tr>
<td>Normal</td>
<td>16111</td>
<td>2298</td>
<td>0.2500</td>
<td>27.4</td>
</tr>
<tr>
<td>Fine</td>
<td>30187</td>
<td>4498</td>
<td>0.3756</td>
<td>98.7</td>
</tr>
<tr>
<td>Finer</td>
<td>83234</td>
<td>13081</td>
<td>0.3558</td>
<td>1158.3</td>
</tr>
<tr>
<td><strong>TRAPEZOIDAL</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coarser</td>
<td>8305</td>
<td>996</td>
<td>0.3339</td>
<td>12.7</td>
</tr>
<tr>
<td>Coarse</td>
<td>13399</td>
<td>1689</td>
<td>0.3566</td>
<td>29.1</td>
</tr>
<tr>
<td>Normal</td>
<td>21845</td>
<td>3064</td>
<td>0.3656</td>
<td>113.6</td>
</tr>
<tr>
<td>Fine</td>
<td>45315</td>
<td>6560</td>
<td>0.2509</td>
<td>551.8</td>
</tr>
<tr>
<td>Finer</td>
<td>119717</td>
<td>18594</td>
<td>0.3401</td>
<td>5239.1</td>
</tr>
<tr>
<td><strong>SQUARE (2mm)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coarser</td>
<td>6729</td>
<td>769</td>
<td>0.3080</td>
<td>9.2</td>
</tr>
<tr>
<td>Coarse</td>
<td>10425</td>
<td>1273</td>
<td>0.2944</td>
<td>17.7</td>
</tr>
<tr>
<td>Normal</td>
<td>19148</td>
<td>2563</td>
<td>0.3498</td>
<td>56.2</td>
</tr>
<tr>
<td>Fine</td>
<td>29260</td>
<td>4144</td>
<td>0.3696</td>
<td>149.8</td>
</tr>
<tr>
<td>Finer</td>
<td>83845</td>
<td>12718</td>
<td>0.3422</td>
<td>1891.2</td>
</tr>
<tr>
<td><strong>SQUARE (1.5mm)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coarser</td>
<td>7496</td>
<td>937</td>
<td>0.3230</td>
<td>12.7</td>
</tr>
<tr>
<td>Coarse</td>
<td>14962</td>
<td>1867</td>
<td>0.2823</td>
<td>42.3</td>
</tr>
<tr>
<td>Normal</td>
<td>31808</td>
<td>4509</td>
<td>0.3195</td>
<td>241.5</td>
</tr>
<tr>
<td>Fine</td>
<td>56461</td>
<td>8369</td>
<td>0.3868</td>
<td>908.5</td>
</tr>
<tr>
<td>Finer</td>
<td>158145</td>
<td>24959</td>
<td>0.2715</td>
<td>17592.2</td>
</tr>
</tbody>
</table>

### 4. Results & Discussions

Pressure lines graphics were plotted for each profile studied. For one predetermined channel length, \( y =3.50\text{mm} \), six pressure lines were plotted at the GDL interior and one at the channel outlet (0.05mm from the upper surface of the channel), in order to evaluate the pressure gradient there. The pressure gradient behavior of the studied models provides homogeneity of the reactants gas flux data through diffusion layer. A homogeneous pressure gradient means higher gas availability for the fuel cell reactions.

According to the graphics shown, a huge stagnation region (dead zone) is noticed at the top of rib between the 2mm square profile channels. In Figure 8 this effect is noticed from the inexistence of a high pressure gradient at 2.50mm < \( x < 3.50\text{mm} \) range (every pressure lines were close to zero).
The 1.5 square profile presents stagnation, but it is local surrounding \( x=1.75 \text{mm} \) (Figure 9).

The trapezoidal and triangular profile channels presented similar responses about pressure gradient throughout the geometry, with no stagnation zones.

![Figure 6: Pressure lines of triangular profile.](image6)

![Figure 7: Pressure lines of trapezoidal profile.](image7)

![Figure 8: Pressure lines of 2mm square profile.](image8)

In the Figures 10-13 the \( z \)-velocity slice profiles for all channels configurations are showed.

At velocity slice graphic (Figure 12) of 2mm square profile, there is a remarkable region of low velocity in \( z \), confirming the obtained results by pressure lines.

Although both triangular and trapezoidal profiles presented pressure gradient (\( \Delta p \approx 0.55 \text{ kPa at GDL} \)) below of the 1.5mm square profile (\( \Delta p \approx 0.65 \text{ kPa at GDL} \)), the \( z \)-direction velocity profile stood around 0.2 m.s\(^{-1}\) throughout \( x \)-axe; the square profiles, instead, presented areas or spots of large velocity decreasing (hitting 0.1 m.s\(^{-1}\) at diffusion layer outlet, \( z=2.25 \text{mm at 2mm square profile and } z=1.75 \text{mm at 1.5 square profile} \)).

In order to check the studied models correspondence within fuel cell experiments, both square profiles (graphite plates) were used.

The polarization curve measures the fuel cell performance in terms of potential, under different values of current. The value of 0.6V (work potential), is set to compare two different fuel cells performance.
In Figure 14 the polarization curves of both prototypes were presented. The values for work operation were: 166.7 mA cm$^{-2}$ and 470.6 mA cm$^{-2}$, for the prototype 1 and 2, respectively.

The graphite plate in prototype 2 had better performance than in the prototype 1, which was validated by numeric methods. Such behavior was attributed to the higher channel area in contact with gas diffusion electrode which provides higher active area available for the gas reaction. Besides the area, higher gas velocities in flow fields decrease the gas stagnation points along the channels.
5. Conclusions

The CFD techniques help the fuel cell’s researchers to explore the connection between the transport of reactants and products and overall cell performance. CFD simulates hydrogen gas flow channels to reduce the costs of bipolar plates’ production through optimization of the mass transport. New geometries are proposed and tested at laboratory scale.

Several models’ simulations of diffusion in porous media and conduction/convection processes were studied. Then, the experimental data were used to visualize the differences in performance between PEMFC 1 and 2. The graphite plate in prototype 2 exhibited better performance than in prototype 1, which was validated by numeric methods. Such behavior was attributed to the higher channel area in contact with gas diffusion electrode which provides higher active area available for the gas reaction. Besides the area, higher gas velocities in flow fields decrease the gas stagnation points along the channels.

6. Acknowledgements

This work was supported by IPEN/CNEN-SP at PROCEL laboratories.

7. References