2007 International Nuclear Atlantic Conference - INAC 2007
Santos, SP, Brazil, September 30 to October 5, 2007
ASSOCIAÇÃO BRASILEIRA DE ENERGIA NUCLEAR - ABEN
ISBN: 978-85-99141-02-1

MODELLING AND SIMULATION OF PEM FUEL CELL´S FLOW CHANNELS USING CFD TECHNIQUES

Edgar F Cunha[1], Alexandre B Andrade[1], Eric Robalinho[1]
Martha L M Bejarano[1], Efraim Cekinski[2] and Marcelo Linardi[1]

[1] Instituto de Pesquisas Energéticas e Nucleares (IPEN / CNEN - SP)
Av. Professor Lineu Prestes 2242
05508-000 São Paulo, SP
efcunha@ipen.br
abodart@ipen.br
eric@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 Proton Exchange Membrane Fuel Cell (PEMFC) consists of two important parts: the Membrane Electrode Assembly (MEA), where the reactions occur, and the flow field plates. The plates have many functions in a fuel cell: distribute reactant gases (hydrogen and air or oxygen), conduct electrical current, remove heat and water from the electrodes and make the cell robust. The cost of the bipolar plates corresponds up to 45% of the total stack costs. The Computational Fluid Dynamic (CFD) is a very useful tool to simulate hydrogen and oxygen gases flow channels, to reduce the costs of bipolar plates production and to optimize mass transport. Two types of flow channels were studied. The first type was a commercial plate by ELECTROCELL and the other was entirely projected at Programa de Célula a Combustível (IPEN/CNEN-SP) and the experimental data were compared with modelling results. Optimum values for each set of variables were obtained and the models verification was carried out in order to show the feasibility of this technique to improve fuel cell efficiency.

1. INTRODUCTION

Nowadays, the need to obtain clean and abundant energy in our world is one of the most concerns of the researches. Fuel cell becomes a promising candidate to obtain this energy from renewable resources, having high power density capability offering low to zero environmental impact. In this scenery, Proton Exchange Membrane Fuel Cell (PEMFC, also called Polymer Electrolyte Membrane Fuel Cell) converts chemical energy directly into electrical energy and heat.

PEMFC works at low temperature, 60-80 °C, with high power density. These properties are ideal for portable applications, such as cell phones and computers; stationary applications, like houses, hospitals or buildings; and automotive applications, cars and busses, for example.

The PEMFC is an electrochemical device and consists of two main parts: The first part is an electrolyte between two gas diffusion electrodes (GDE), an anode and a cathode with two gas diffusion layers (GDL). This structure is called Membrane Electrode Assembly (MEA). The second part is the gas flow field plates, called bipolar plates, in the case of a stack. The

bipolar plates have many functions in a fuel cell [1]: distribute reactant gases (hydrogen and air or oxygen) uniformly, collect and conduct electrical current, besides remove heat and water from the electrodes. The bipolar plates make the cell robust and rigid to support the impacts of portable and automotive applications. The cost of the bipolar plates corresponds up to 45% of the total stack costs and about 80% of the total weight of the stack [2, 3].

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 [4-6].

Mathematical modeling is a very important part of the actual research and development work in science and engineering. In fact competitive research requires speed on path between idea and prototype, and mathematical modeling and simulation provides a valuable shortcut for understanding qualitative and quantitative aspects of scientific design.

In this work, two flow channels configurations by simulation with COMSOL software were studied and a preliminary experimental test to verify the model applied in these configurations was conducted.

2. METHODOLOGY

Two single cells of 144 cm² of active area were manufactured, called prototype 1 by ELECTROCELL, and prototype 2 by IPEN. The serpentine flow field for channel geometry was chosen. The configuration of flow field in the prototype 1 was: 2 mm width and 2 mm deep 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 deep channels and 0.5 mm ribs. For this prototype, each part of serpentine flow field was composed by 12 channels and 11 ribs.

For these flow field configurations, the channel area of the prototype 2 was 0.110 m^2 and 0.073 m^2 for prototype 1. In Fig. 1 (a) and (b) the bipolar plates for prototypes 1 and 2 were showed, respectively.

(a)  (b) 

Figure 1. (a) Flow field channels from prototype 1 and (b) prototype 2.

The best-known membrane 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 electrocatalysts; and two gas diffusion layers, like carbon paper or carbon cloth.

For these experiments ETEK MEA's with active area of 144 cm^2, double side ELAT electrodes were used. The electrodes, anode and the cathode, with 20 % Pt on Vulcan XC-72, and platinum loadings of 0.4 mg Pt cm^{-2} were built. Nafion™ 115 membrane as electrolyte was used.

Fuel cell polarization measurements were carried out galvanostatically with the single cell at 70 °C, using oxygen and hydrogen with satured water vapor (Millipore quality – Elix 3 model) at 85 °C, atmospheric pressure and hydrogen volumetric flux 8.33 10^{-6} m^3 s^{-1}. The entrance areas for prototype 1 and prototype 2 were 6.0 10^{-6} m^2 and 2.25 10^{-6} m^2, respectively.

The flow distribution is described by two equations: Navier-Stokes (Eq.1.) and continuity (Eq.2.),

$$r\frac{\partial u}{\partial t} - \nabla . h\left(\nabla u + (\nabla u)^T\right) + r(u.\nabla)u + \nabla p = 0 \quad (1)$$

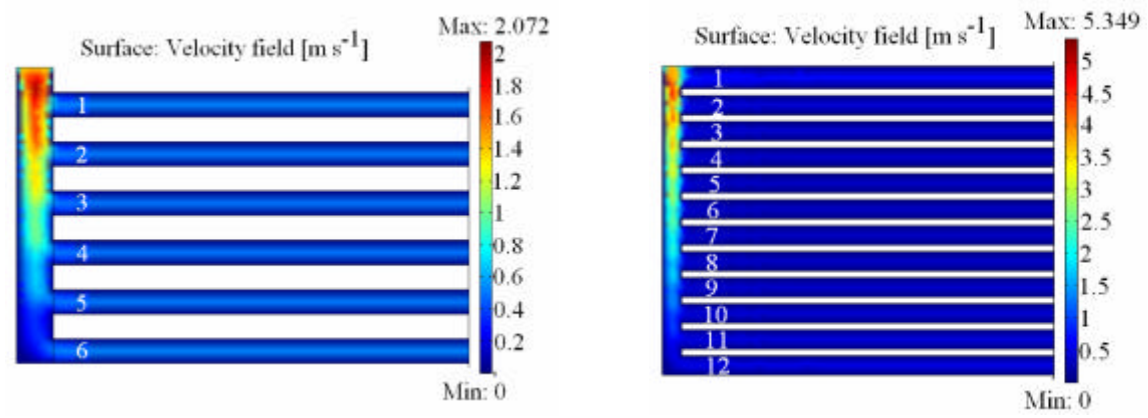
$$\nabla . u = 0 \quad (2)$$

where r denotes the density [kg m^{-3}], **u** the velocity vector [m s^{-1}], h 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 solver used Direct UMFPACK with Elimination constraint handling method over a mesh with more than 200.000 degrees of freedom, at 3.2GHz Pentium IV PC with 3GB RAM..

3. RESULTS AND DISCUSSION

The velocity magnitude throughout the field channels was studied. To design the channels and simulate the velocity profiles, the COMSOL Multiphysics software was used. In this case a 2D geometry was chosen. The models in 2D geometry are lighter and faster to simulate and represent a good resolution for evaluating the flow behavior.

In Fig. 2, details of the gas entrance in the first part of the serpentine flow field for (a) prototype 1 and (b) for prototype 2 are showed.

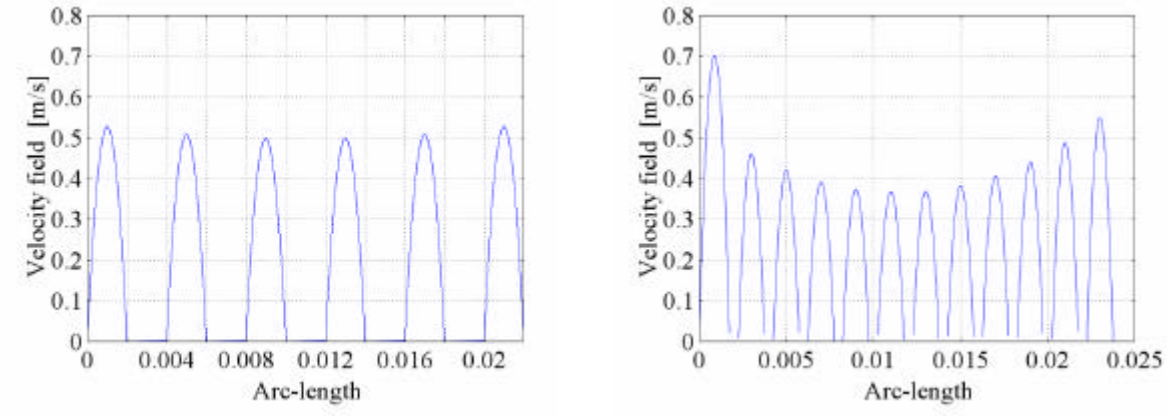


(a) (b)

Figure 2. Velocity flow fields: (a) prototype 1 and (b) prototype 2.

The first channel, number 1 in Fig. 2 (a) and (b), is the nearest of gas entrance. Because the gas entrance and channel areas of prototype 1 are bigger than prototype 2, different velocity values were obtained.

In Fig. 3 the velocity profiles in the middle of the first set of the serpentine path for (a) prototype 1 and (b) for prototype 2 are showed. Each channel is represented by one peek.



(a) (b)

Figure 3. Velocity profiles in each channel: (a) prototype 1 and (b) prototype 2.

In Fig. 3 (a) and (b), with the same volumetric flux conditions, more homogeneous velocity profiles distribution in the prototype 1 was observed. In these simulations a parabolic velocity profiles that corresponding to laminar flow were obtained.

In Tab. 1 the numbers of elements and degrees of freedom are showed. The complex geometry of the prototype 2 demands more elements in its associated mesh, and more time to converge the solution.

Table 1. Elements and degrees of freedom for 2D modelling

	Prototype 1	Prototype 2
Elements	27486	33568
Degrees of freedom	218449	265058

3.2. Fuel Cell Polarization Measurements

An experimental test with the prototypes was carried out. The performance of the fuel cell was measured by polarization curves. The polarization curves were taken in steady state conditions and represent the behavior of the fuel cell potential versus current density. In Fig. 4 the comparison of the polarization curves for both prototypes is showed.

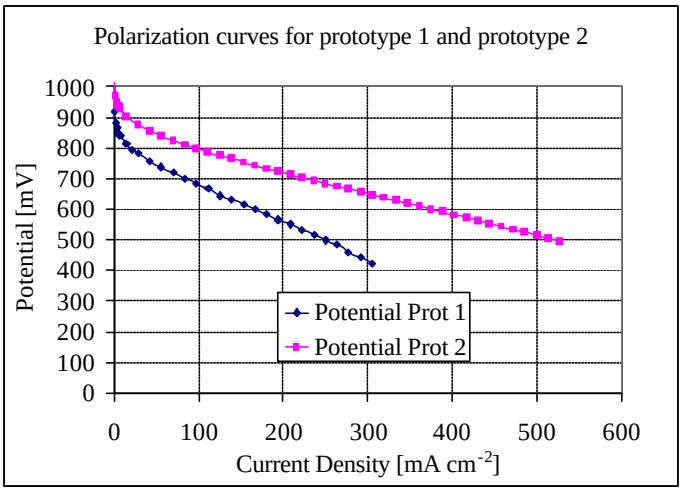


Figure 4. Comparison of the performance for prototypes 1 and 2.

In general, the performance of fuel cells is compared at 600 mV potential, usually chosen as the operating potential. At this potential, current densities of 166 mA cm^{-2} and 375 mA cm^{-2} for prototype 1 and 2 were obtained, respectively. For practical applications, one single cell is not enough to supply any practical device, so several single cells are assembled in series, making a stack. In this case, a high current density is required to obtain a stack with few single cells, consequently lighter and cheaper.

4. CONCLUSIONS

A primary simulation of flow field channels was performed and the velocity profiles were calculated. In prototype 1, the velocity profiles were more homogeneous than prototype 2. An accurate model including other processes, like diffusion and reactions, could simulate dead zones, water management and reagents and products distribution, evaluating a better solution.

In the experiments, a better performance of prototype 2 was obtained. This result was due to the higher channel area in contact with gas diffusion electrode and consequently more active area available for the gas reaction. Besides the area, higher gas velocities in flow fields decrease the gas stagnation points along the channels.

For future works, simulation with 3D geometry will be studied and other processes, like the diffusion in porous media and electrochemical reactions will be considered.

ACKNOWLEDGMENTS

This work was supported by IPEN/CNEN-SP at PROCEL laboratories. The authors would like to thank ELECTROCELL and FEI (Fundação Educacional Inaciana) by manufacturing of the bipolar plates.

REFERENCES

1. E. Middelman, W. Kout, B. Vogleaar, J. Lenssen, E. de Waal, ''Bipolar plates for PEM fuel cells,“ *Journal of Power Sources*, **Volume 118**, pp.44-46 (2003)

2. A. Kummar, R. G. Reddy, ''Materials and design development for bipolar/end plates in fuel cell,“ *Journal of Power Sources*, **Volume 129**, pp.62-67 (2004)

3. W. Quian, D. P. Wilkson, J. Shen, H. Wang, J. Zhang, “Architecture for portable direct liquid fuel cells”, *Journal of Power Sources*, **Volume 154**, pp.202-213 (2006)

4. P. T. Nguyen, T. Berning, N. Djilali, ''Computational model of PEM fuel cell with serpentine gas flow channels,“ *Journal of Power Sources*, **Volume 130**, pp.149-157 (2004)

5. S. Karvonen, T. Rottinen, J. Saarinen, O. Himanen, ''Modeling of flow field in polymer electrolyte membrane fuel cell,“ *Journal of Power Sources*, **Volume 161**, pp.876-884 (2006)

6. G. Squadrito, O. Barbera, I. Gatto, G. Giacoppo, F. Urbani, E. Passalacqua, ''CFD analysis of the flow field scale-up influence on the electrodes performance in a PEFC,“ *Journal of Power Sources*, **Volume 152**, pp.67-74 (2005)