



24th COBEM - 2017



24th ABCM International Congress of Mechanical Engineering
December 3-8, 2017, Curitiba, PR, Brazil

COBEM-2017-1479

INFLUENCE OF ELECTRODE FLOW CHANNEL CHANGES ON THE EFFICIENCY OF POLYMER ELECTROLYTE FUEL CELL

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Abstract. Growing concern about environmental impacts and the depletion of fossil fuel sources has motivated the research of new forms of energy derived from renewable sources. In this context, in which the main focus is to mitigate the environmental pressures, this article presents as an option the use of fuel cell technology, that obtains water and energy from gases such as hydrogen and oxygen and don't generate pollutants during the process. This paper analyzes the influence of electrode flow channel changes on the efficiency of polymer electrolyte fuel cell. The research methodology integrates computational fluid dynamic (CFD) and design of experiments (DOE) with the objective of approaching and quantifying operational parameters of greater relevance for cell efficiency with different profiles of flow channels of the electrodes. For this reason, it carries out a comparative study between different fields of flow acting on the anode flow channel changes and setup.

Keywords: Anode, Proton Exchange Membrane Fuel Cell, prototypes

1. INTRODUCTION

The fuel cell is an electrochemical device that converts chemical energy into electrical energy by being fed by gaseous hydrogen and an oxidizing agent, which may be either oxygen gas or atmospheric air. The operating principle is similar to batteries, with the difference that its reactants are stored externally to the devices and the supply is carried out continuously. The reaction mechanism consists of the injection of hydrogen gas at the anode where the electrochemical reactions are initiated at the interface electrode / catalyst / electrolyte and cathode on the other side is injected in the atmospheric air or oxygen. The ions formed at the anode interface have their passage made to the cathode through the electrolyte. Meanwhile, the electrons generated in the anode half reaction are transported through an external circuit to the cathode. The fuel cell which uses a solid electrolyte polymer which carries ionic conduction when hydrated is called Proton Exchange Membrane Fuel Cell. The study of the efficiency of this cell type is associated with the correct hydration of the membrane and optimization of current density.

2. FLOW CHANNEL

The geometry of the large flow channels has influence on the energy efficiency of the fuel cell; these are the channels of the anode or cathode (PAULINO, 2004). On the anode side, the flow channels are responsible for transporting and distributing the fuel through the diffuser layer of the gas. The literature suggests that the most relevant study relates to water accumulation in the channels, many of the time becomes one of the causes of loss of efficiency because the excess water molecules causes the hydrogen protons are blocked before of the electrochemical reaction to generate electricity. The water accumulation be more evident in the cathode where water is effectively generated by hydrogen bond with oxygen from the air, which is inserted in the channel, it can also occur at the anode due to water generated in the cathode flooding the cell to the anode. When it has a suitable geometry for a given water removal rate, the excess can be avoided and therefore the reagents occurs without transport blocks (BELCHOR, STRONG and

CARPENTER, 2012). In the case of fuel cells, the complexity involved in and electric production process is influenced by several factors, among them is the geometry of the channels. In order to understand the contribution of these various factors, it is used as a tool to computer simulation of fluid - CFD associated with the design of experiments. The literature demonstrates that changes in channel geometries can be performed in different ways (CHANG and HUNG, 2012). The article discusses the modifications in the configuration of the anode channels. The basic model uses an interstitial configuration, turn the prototypes 1, 2 use the settings in parallel and coil, respectively. Finally, prototype 3 will use a specific configuration proposed in this article.

2.1 Equations

The electrochemical cell kinetics is described by the Butler-Volmer equation shown in Equation 1.

$$i = i_0 \left[\exp \left(\frac{-\alpha_a z F}{RT} \eta \right) - \exp \left(\frac{\alpha_c z F}{RT} \eta \right) \right] \quad (1)$$

Where current density is influenced by reagent concentration and pressure and temperature operation of the cell. The parâmetro η is given by the difference between the cell potential and the equilibrium potential, according to Equation 2.

$$\eta = (E - E_{eq}) \quad (2)$$

In the flow channels, the gas flow is governed by the Navier-Stokes equation, considering the fluid as incompressible.

$$\nabla \cdot (\rho u) = 0 \quad (3)$$

$$\rho u \cdot \nabla u = -\nabla \cdot (-pI + \tau) \quad (4)$$

$$\tau = \mu[\nabla u + (\nabla u)^T] - \frac{2}{3} \mu(\nabla \cdot u)I \quad (5)$$

The concentration of water is represented by the equation 6 and 7.

$$\lambda = 0,043 + 17.18a - 39.85a^2 + 36a^3 (a < 1) \quad (6)$$

$$\lambda = 14 + 1.4(a - 1)(a > 1) \quad (7)$$

Where parameter is found by the Equation 8 represents the relationship between vapor pressure and saturation pressure

$$a = \frac{P_{wv}}{P_{sat}} \quad (8)$$

3. DESIGN OF EXPERIMENTS

The methodology known as Experiment Design, DOE - Design of Experiments, was introduced by Fisher in 1935 and initially applied to experiments in agriculture, biology and quality engineering. This statistical technique is used to relate the study variables, which are entries in the development of products and processes, the output variables, which are system responses (MONTGOMERY, 1997). In making this relationship, the influence of the input parameters on the output variables is identified, noting the most sensitive points that can be controlled. The Project of experiments is operationalized through computer programs, which manage to the data collected and establish the relationship between the input data and response variables. When developing an experiment of a product or process the input variables that can be controlled must be known. The controlled parameter gives the name of factors and assumed values of each variable are given the name of level. The study of the set formed by factor, level and variable of response allows to qualitative analysis by determining the variables that influence the response variable and quantitative analyzes demonstrating how much the input variables are related to the response variables. In this article we will be presented an integration of the analysis of variance using Fischer-Snedecor test statistic of Tukey's test and conducting a qualitative analysis of the cell.

3.1 Analysis of Variance - ANOVA

Analysis of variance (ANOVA) tests the hypothesis that the mean of two or more populations are equal. ANOVA evaluates the importance of one or more factors, comparing the average response variables at different levels of factor. The null hypothesis states that all averages population share are equal while the alternative hypothesis states that at least one is different. The procedure works by comparing the variance between the means of groups versus the variance within the groups as a way to determine if the groups are part of a larger population or distinct populations with different characteristics. The indicator to characterize an analysis of variance statistical is F. Therefore F provides a statistical test variable, called F -test to check the acceptance or rejection of the null hypothesis. It is necessary to compare the value of the variable F observed with the critical value of F obtained in the distribution tables F to the desired value of significance. F should be greater than the critical test for a significant, then reject Ho. Table 1 represents an observation x treatment matrix, and the F statistic has its described in equations 9, 10 and 11.

Table 1: Number of observations per treatment

Observation/treatment	1	2	3	G
1	X ₁₁	X ₁₂	X ₁₃	X _{1g}
2	X ₂₁	X ₂₂	X ₂₃	X _{2g}
N	X _{n1}	X _{n2}	X _{n3}	X _{ng}

$$F = ((SQE/g-1)/(SQD/(ng-g))) \quad (9)$$

$$SQE = \sum_{j=1}^g \sum_{i=1}^n (\bar{x}_j - X)^2 \quad (10)$$

$$SQD = \sum_{i=1}^n \sum_{j=1}^g (x_{ij} - \bar{x}_j)^2 \quad (11)$$

SQE: sum of squares between treatments

SQD: sum of squares within treatments

n: sample size of each treatment

g: total number of treatments

\bar{x}_j : Average of each treatment

X: Global average of treatments

x_{ij} : Value of observation

After the calculation of statistic to F - F_{calc}, performs the comparison with the tabulated F - F_{tab}, known as critical F, where Test F is greater than F tabulated demonstrates was found that there is an average gap that needs to be studied. The F-statistic is in Table 2.

Table 2: Statistic F – Snedecor

ng-g	g -1								
	2	3	4	5	6	7	8	9	10
5	5,79	5,41	5,19	5,05	4,95	4,88	4,82	4,77	4,74
6	5,14	4,76	4,53	4,39	4,28	4,21	4,15	4,10	4,06
7	4,74	4,35	4,12	3,97	3,87	3,79	3,73	3,68	3,64
8	4,46	4,07	3,84	3,69	3,58	3,50	3,44	3,39	3,35
9	4,26	3,86	3,63	3,48	3,37	3,29	3,23	3,18	3,14
10	4,10	3,71	3,48	3,33	3,22	3,14	3,07	3,02	2,98
11	3,98	3,59	3,36	3,20	3,09	3,01	2,95	2,90	2,85
12	3,89	3,49	3,26	3,11	3,00	2,91	2,85	2,80	2,75

3.2 Tukey Test

The F test indicates whether there is a difference between the measured the treatments, however, does not indicate the best treatment. In this case, it is necessary to apply a test mean comparison of treatments, may then conclude that the best treatment. Then the average comparison tests serve as a complement to the study of analysis of variance. There are several means of comparison tests, among which we can mention the Tukey test. Tukey's test has as a reference the least significant difference - DMS represented by Equation 12. After calculating the DMS the value obtained by the Tukey test is compared to the difference obtained between the general mean and the mean of each treatment. If the test value is less than the value found from the difference between averages, it means that the study treatment makes a significant difference, the input variable under study influence the output variable as equation 12 and 13.

$$DMS = q * \left(\frac{SQD / (ng - g)}{n} \right)^{\frac{1}{2}} \quad (12)$$

$$\| \bar{x}_j - X \| > DMS \quad (13)$$

Table 3 is a table of illustration Tukey which allows finding the parameters q (g, ng-g).

Table 3: Tukey Test

ng-g	g								
	2	3	4	5	6	7	8	9	10
5	3,64	4,6	5,22	5,67	6,03	6,33	6,58	6,8	6,99
6	3,46	4,34	4,9	5,3	5,63	5,9	6,12	6,32	6,49
7	3,34	4,16	4,68	5,06	5,36	5,61	5,82	6	6,16
8	3,26	4,04	4,53	4,89	5,17	5,4	5,6	5,77	5,92
9	3,2	3,95	4,41	4,76	5,02	5,24	5,43	5,59	5,74
10	3,15	3,88	4,33	4,65	4,91	5,12	5,3	5,46	5,6
11	3,11	3,82	4,26	4,57	4,82	5,03	5,2	5,35	5,49
12	3,08	3,77	4,2	4,51	4,75	4,95	5,12	5,27	5,39

4. RESULT AND DISCUSSION

From this reference model, it was possible to elaborate other three prototypes with different geometry and arrangement, Thus making the comparison and verifying the possible or not, an in the improvement performance of this PEM - Proton exchange fuel cell. Therefore, if the changed geometry of the anode channels with intentions will check its influence on the determination of the amount of water and the current density of the cell. These physical quantities will be verified through experimental design and computational dynamic fluid. The models developed are located in figures 1, 2, 3 and 4.

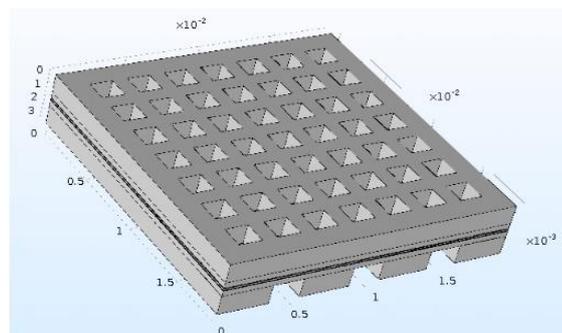


Figure 1 – Base prototype

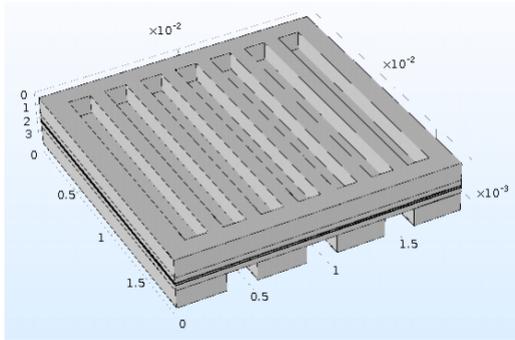


Figure 2 – Prototype 1

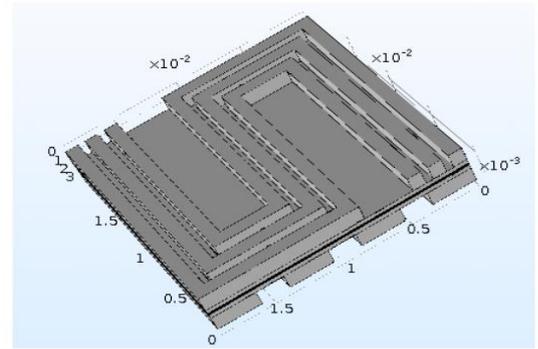


Figure 3– Prototype 2

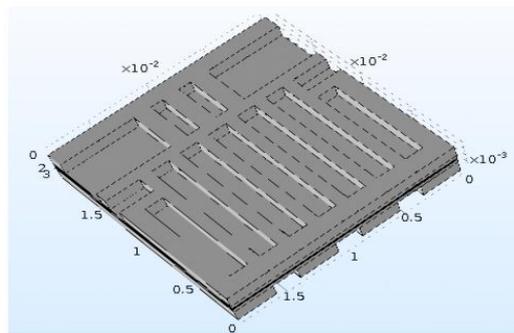


Figure 4 – Prototype 3

4.1 Simulation Condition

The simulation conditions are in Table 04.

Table 4: Simulation Conditions

Nomenclature	Value [Unit]	Description
eps_gdl	0,4	GDL porosity
kappa_gdl	1.18e-11[m^2]	GDL permeability
sigma_gdl	222[S/m]	GDL electric conductivity
wH2_in	0,743	Inlet H2 mass fraction (anode)
wH2O_in	0,023	Inlet H2O mass fraction (cathode)
wO2_in	0,228	Inlet oxygen mass fraction (cathode)
mu_anode	1.19e-5[Pa*s]	Anode viscosity
mu_cathode	2.46e-5[Pa*s]	Cathode viscosity
MH2	0.002[kg/mol]	Hydrogen molar mass
MN2	0.028[kg/mol]	Nitrogen molar mass
MH2O	0.018[kg/mol]	Water molar mass
MO2	0.032[kg/mol]	Oxygen molar mass
T	180+273.15[K]	Cell temperature
p_ref	101e3[Pa]	Reference pressure
V_cell	0,9	Cell voltage
cO2_ref	40.88[mol/m^3]	Oxygen reference concentration
cH2_ref	40.88[mol/m^3]	Hydrogen reference concentration
sigma_m	9.825[S/m]	Membrane conductivity

4.2 Design of experiments

The statistical survey was conducted in each prototype, with the aim of meeting the F statistic and analyzes the Tukey test. First he obtained the current density in membrane models and, in a second step the obtained off water concentration values in the anode according to Tables 5 and 6. We used 26 sample points for each of the four treatments.

Table 5: Current density (A/m^2)

A/m^2	X	\bar{x}_i	F_{calc}	F_{tab}	DMS	$X - \bar{x}_i$
Base Prototype	$6,5*10^3$	$6,2*10^3$	0,02	2,69	NA	NA
Prototype 01		$6,4*10^3$				NA
Prototype 02		$6,7*10^3$				NA
Prototype 03		$6,7*10^3$				NA

For the current density F_{calc} is less than F_{tab} . Thus, there is no significant difference between the averages that needs to be analyzed. Therefore, does not apply (NA) Tukey's test to determine which model generated a difference in current density with the change of cell geometry.

Table 6: Concentration of water at the anode (mol/m^3)

mol/m^3	X	\bar{x}_i	F_{calc}	F_{tab}	DMS	$X - \bar{x}_i$
Base Prototype	1,26	1,06	1,31	2,69	NA	NA
Prototype 01		1,06				NA
Prototype 02		1,85				NA
Prototype 03		1,06				NA

For the water concentration is less than $F_{calc} F_{tab}$. Thus, there is no significant difference between the averages that needs to be analyzed. Therefore, not applicable (NA) Tukey's test to determine which model generated a difference in water concentration with the change in geometry of the cell. The mean values are close because the geometry change occurred only in the anode. The higher effect on water concentration occurs in the cathode due to its production in the chemical reaction carried out in the cell.

4.3 Gradient current density and concentration of water

The realization of the experimental design with the tools discussed in this article allows the researcher to perform a qualitative analysis of the fuel cell. In order to study complement representation of the current density gradient in the membrane and the concentration of water at the anode in continuous operation was carried out. The current density maps are shown in Figures 5, 6, 7 and 8.

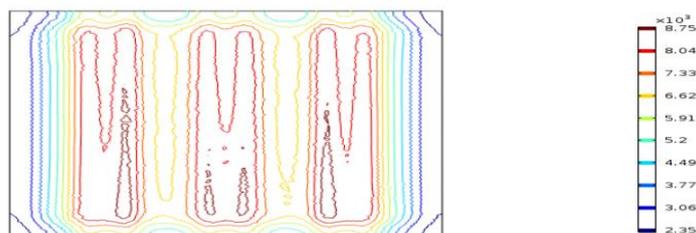


Figure 5 – Current density model based

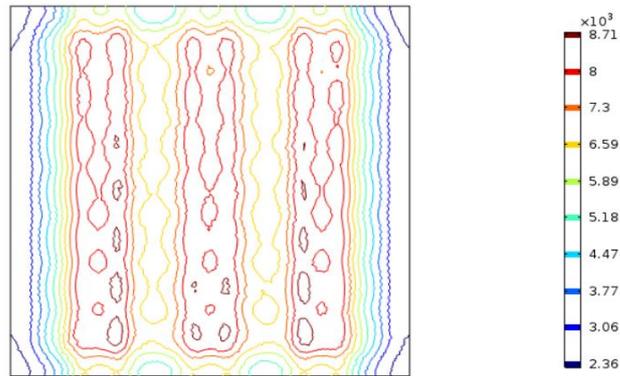


Figure 6 – Current density prototype 1

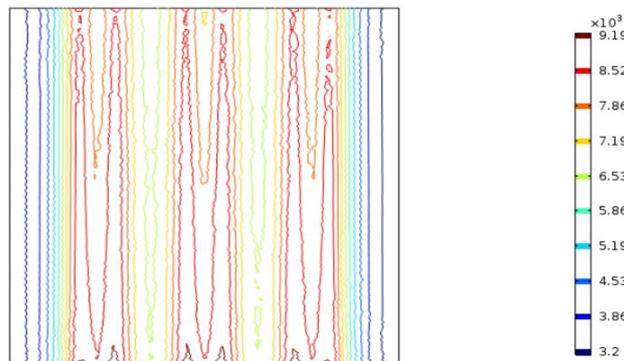


Figure 7 – Current density prototype 2

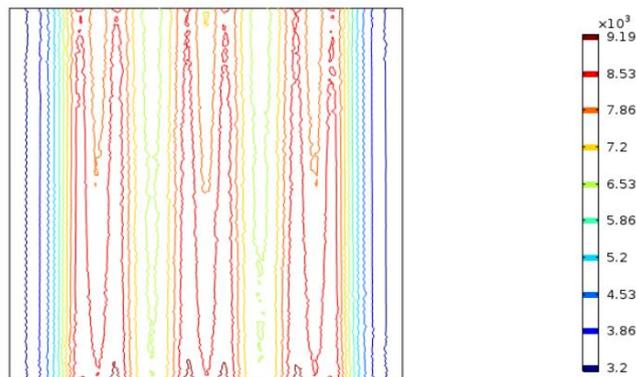
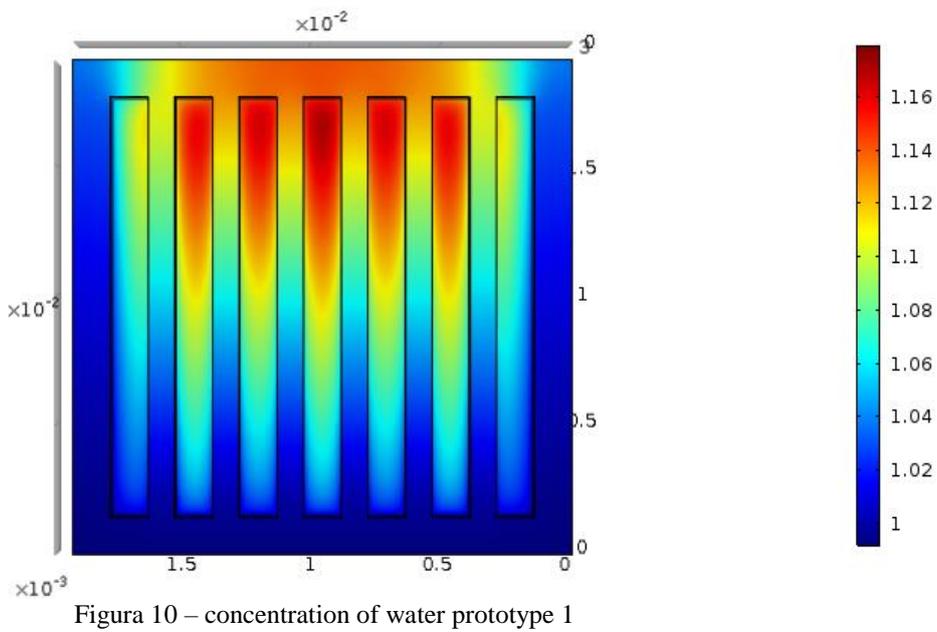
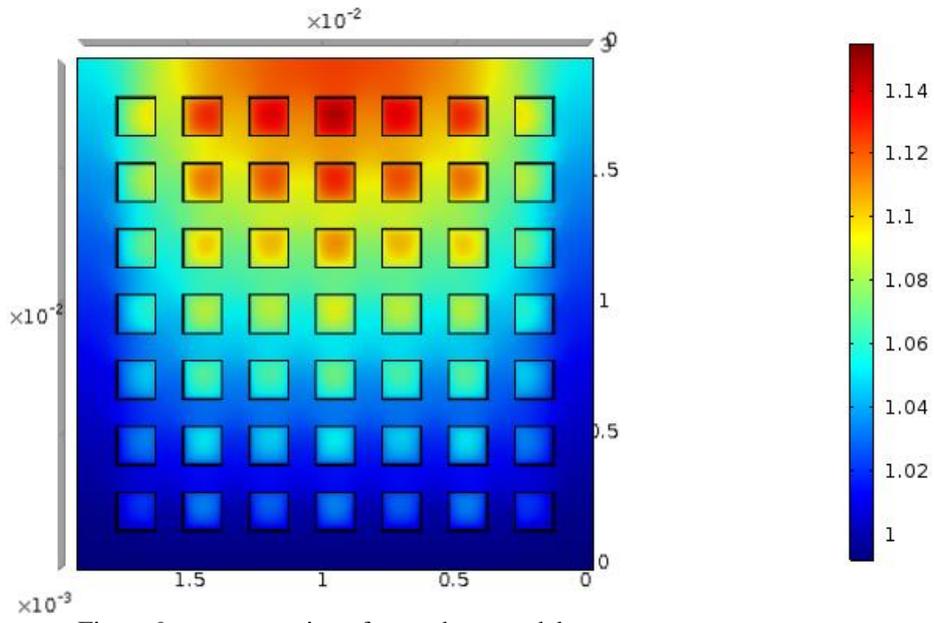


Figure 8 – Current density prototype 3

Note that the current density of the membrane was very similar models studied. It is observed that the lower current density values are in the regions opposed to the cathodes channels. In turn, the higher current density values are in the region between the cathode channels. Prototypes 2 and 3 showed the highest current density in the membrane. The maps of concentration of water in the anode are shown in Figures 9, 10, 11 and 12.



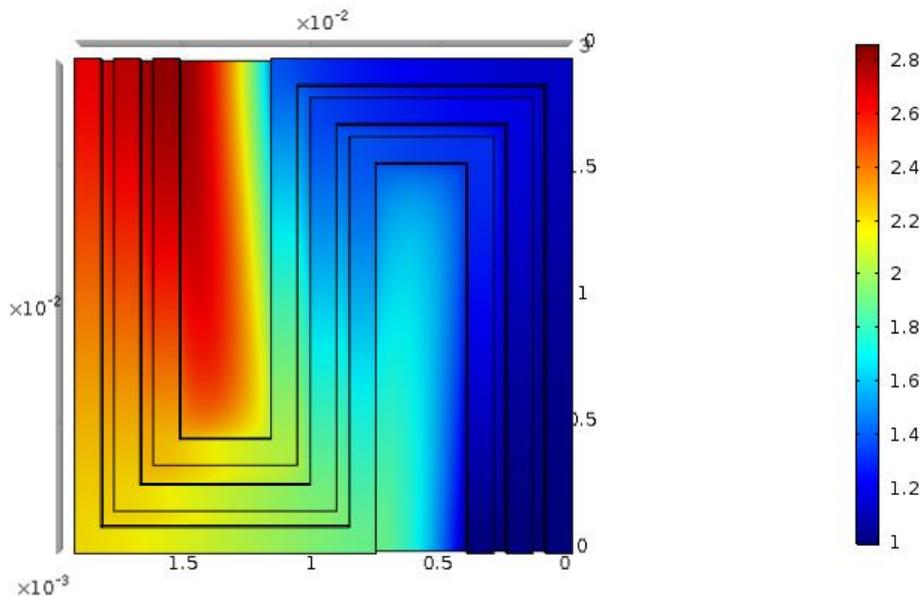


Figure 11 – concentration of water prototype 2

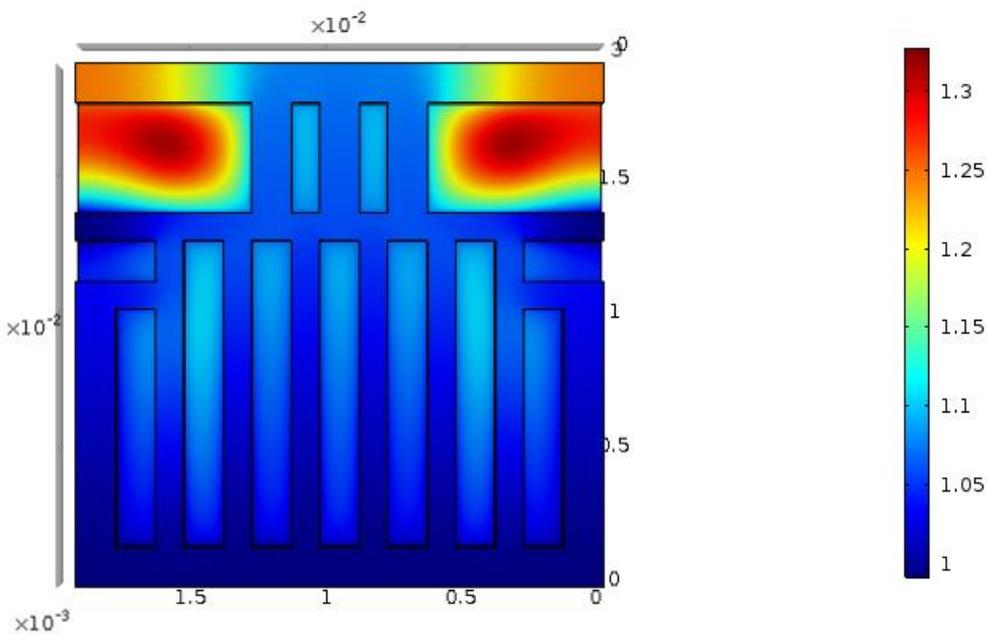


Figure 12 – Concentration of water prototype 3

Comparing the concentration of water in the prototypes 1, 2 and 3 in relation to the basic model, it is observed that the prototype 1 presents a more linear distribution. Prototype 2 showed a distribution that divides the cell, but concentrates the highest levels in the output channel. In turn, the prototype 3 in question fell saturation of the catalyst.

5. CONCLUSION

It is observed that when performing the statistical treatment in line with the computational dynamic fluid tool it is possible to obtain a greater reliability in the data studied through statistical tables that present a confidence index of the sample. The design of experiments is presented as a viable alternative in the reduction of research times, since it allows to discover the influences of the input variables in the desired outputs for the product being studied. The statistical treatment addressed in this article did not present a significant difference in the variables of current density and water concentration, showing that only changes in the anode channels do not present a relevant influence on these cell parameters.

6. REFERENCES

- BELCHOR, P. M.; FORTE, M. M. C.; CARPENTER, D. E. O. S. Parallel serpentine-baffle flow field design for water management in a proton exchange membrane fuel cell. *International Journal of Hydrogen Energy*, v. 37, n. 16, p. 11904–11911, Agosto 2012.
- CHANG, D.-H.; HUNG, J.-C. Effects of Channel Depths and Anode Flow Rates on the Performance of Miniature Proton Exchange Membrane Fuel Cells. *International Journal of Applied Science and Engineering*, v. 4, p. 273280, Outubro 2012.
- MONTGOMERY, D. C. (1997), *Design and Analysis of Experiments*, John Wiley and Sons: New York.
- PAULINO, A. L. D. R. Estudo da Geometria de Canais de Fluxo em Células a Combustível Tipo PEMFC Utilizando Fluidodinâmica Computacional. INEP - Instituto de Pesquisas Energéticas e Nucleares. São Paulo, p. 84. 2014.

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