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MODELING AND PARAMETRIC ANALYSIS OF PEM FUEL CELLS USING COMPUTATIONAL FLUID DYNAMICS

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Abstract. *This paper presents a parametric investigation of PEMFC electrochemical models employing computational fluid dynamics (CFD) technique and aims to determine the relative importance of each parameter on the modeling results. A compatible and systematic mathematical model is developed in order to study the effect of these parameters. The model is applied to an isothermal, steady state an single phase to observe the main results by a polarization curve. The results compare well with the experimental polarization data obtained at 80 ºC for ohmic and activation regions. The best match with the experimental data is obtained when the specific active surface area of the catalyst layer is 700 cm^2/mg and electrolyte conductivity of 8 S/m.*

Keywords: *CFD, PEM fuel cell, fuel cell modelling, numerical simulation*

1. INTRODUCTION

The objective of this work is to demonstrate the importance of the computational simulation used in fuel cells, which can, for example, study several components such as: flow channels, membranes, catalyst layer, gas diffusion layer or bipolar plates. The main objective is to present parametrization techniques in order to construct a polarization curve simulate closer to the experimental data. Thus, in this study, a PEM fuel cell is numerically modeled, the model is compared with experimental data and the parameters investigated are the specific surface area of the catalyst layer and the effective conductivity of the electrolyte, with future objectives of studying the degradation in these components. Proton exchange membrane fuel cells (PEMFC), are built out of membrane electrode assembly (MEA) which include the electrodes, electrolyte, catalyst, and gas diffusion layers (GDL) and are an interesting alternative for electrical power generation. They operate at low temperatures of about 30 to 100 °C and require catalysts to increase the rate of anode reactions. As fuel, hydrogen or liquid fuel, such as methanol or ethanol is used, and as oxidant the oxygen contained in the air. The bipolar plates have the function to distribute the reagents uniformly on the surface of the diffusion layer by means of flow channels that differ in the constitutions of the geometries implying in strong influence in the final performance of the cells. The materials used in bipolar plates are metals, graphite or carbon-based compounds. When the gaseous hydrogen is used as fuel, it is injected with a certain pressure and flows through the channels until it contacts the platinum-based catalyst at the anode, thereby suffering oxidation and releasing electrons. The ion H formed

by the bond breaking of the hydrogen molecule, bounds to the water molecule forming the hydroxyl ion H_3O^+, also called proton. The ions H_3O^+ are driven by the electric field generated due to the contact with the membrane structure, thus occurring the displacement of electrons through an external circuit with the emergence of a direct current. According to Sezgin et al. (2016) The effect of inlet velocities of air and hydrogen, and the effect of proton conductivity of acid doped PBI membrane, are investigated for a high temperature PEM fuel cell by using Comsol Multiphysics CFD analysis. The authors concluded that the best match with the experimental data is obtained where proton conductivity is 14 S/m, instead of experimental proton conductivity value, 10 S/m. Skoda (2014) presented a study of flow fluids in the cathode channels of a PEMFC fuel cell. Experimental and numerical results were obtained with variations of working temperature and plate flow in parallel channels. The experimental set-up was represented by a transparent cell with the objective of observing the phenomenon of flooding in cathode channels. As a result, it has been shown that the water saturation level increases with decreasing temperature and the experimental polarization and power curves for the oxygen flow rate of 60 $mlmin^{-1}$ and 115 $mlmin^{-1}$ at 25 °C, indicated that performance remained unchanged for this variation of oxygen.
Srinivasulu et al. (2011) reported that the modeling parameters of PEM fuel cell were analyzed using Multi-Parametric Sensitivity Analysis (MPSA). Moreover, finding the definition of the values, for fuel cell simulation parameters, is not a simple task. Acording to authors, using the present work, it is possible to evaluate the importance of each parameter to the simulation accuracy.

Tao et al. (2006) developed a comprehensive review of the mathematical modeling of proton exchange membrane fuel cells. It is found that the results studied by different models in the literature often agree well with the experimental data where, in this first paper a three-dimensional, two-phase and non-isothermal model is investigate, and numerical simulations for a basic case is performed. Siegel (2008) showed a review of modeling strategies and commonly used assumptions in solver implementations, popular numerical algorithms, and computational techniques usually used for fuel cell modeling.

2. COMPUTATIONAL MODELLING METHODOLOGY

Using computational modelling software, it is possible to save some time and expense involved in testing fuel cell designs. For this analysis, modeling and simulation were executed in the commercial software COMSOL Multiphysics 5.2a, which was used to build a single-phase isothermal and tridimensional fuel cell model with finite element method. For this model, the following conditions were assumed: isothermal system, ideal gas mixtures, and compressible model. The principle of simulation was based in the coupling in two reacting flow in porous media, concentrated species interfaces to one secondary current distribution interface. Besides that, the conservation equations are also used in general be represented by the solution of conservation for mass, momentum, species and current transport. In addition, special equations are apply in fuel cell such as:

- Darcy's equation for fluid flow in porous media,
- Stefan-Maxwell equation for multispecies diffusion,
- Faraday Law in electrical current and electrochemical reaction,
- Butler-Volmer equation between electrical current and potential,
- Ohm's law of electrical current conduction.

2.1 General equations

The main equations used in the computational study are those represented by the transport of momentum, species and electric charges. In the moment transport, the use in the flow channels and the porous media is given by the Darcy-Brinkman equation:

$$\frac{\rho}{\epsilon}(\boldsymbol{u}.\nabla)\frac{\boldsymbol{u}}{\epsilon} = \nabla.\left[-P\mathrm{I} + \frac{\mu}{\epsilon}(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T) - \frac{2\mu}{3\epsilon}(\nabla.u)\mathrm{I}\right] - \left(\mu k^{-1} + \beta_F|\boldsymbol{u}| + \frac{Q_m}{\epsilon_p^2}\right)\boldsymbol{u} \quad (1)$$

Where the main terms in Eq. 1 are the density ρ, the velocity vector u, the dynamic viscosity μ, the pressure P, ε is the porosity, k the permeability of the porous media, Q_m is the mass source term. The advection equation was used to calculate the transport fluxes of each species in terms of mass fraction gradients:

$$\nabla.\boldsymbol{J_i} + \rho(\boldsymbol{u}.\nabla)\omega_i = R_i \quad (2)$$

Where ω_i is the mass fraction, J_i represents the diffusion flux vector and R_i represents the reaction rate term of the species. Finally, the electrodes in an electrochemical cell are usually metallic conductors and therefore their voltage-current relationship follow Ohm's law equation:

$$i_s = -\sigma_k \nabla \phi_k \quad (3)$$

Where i is the current density vector (A/m^2), σ_k is the conductivity (S/m), φ_k is the electric potential (V) and Q_k denotes the source term (A/m^3). The subscript k represents l for the electrolyte and s for the electrode respectively.
The model used to describe the kinetics in the electrodes and electrolyte is the linearized Butler-Volmer equation:

$$i_{loc} = i_0 \left[\frac{F}{RT} (\alpha_a + \alpha_c) \right] \eta \quad (4)$$

Where α_{ac} are the cathodic and anodic transfer coefficients (0.5 for both), η is the anodic or cathodic overpotential, F the Faraday constant, R the universal gas constant, i_{loc} is the density local charge transfer current, T the work temperature and i_0 the exchange current density (A / m^2).

3. MODEL DOMAIN

Geometrical parameters and the layers model are shown in Fig. 1 and Fig. 2. The model has 5 cm^2 active area and serpentine single type flow channels. In Table 1 lists the geometrical dimensions of the fuel cells studied and input parameters necessary for simulation are listed in Table 2.

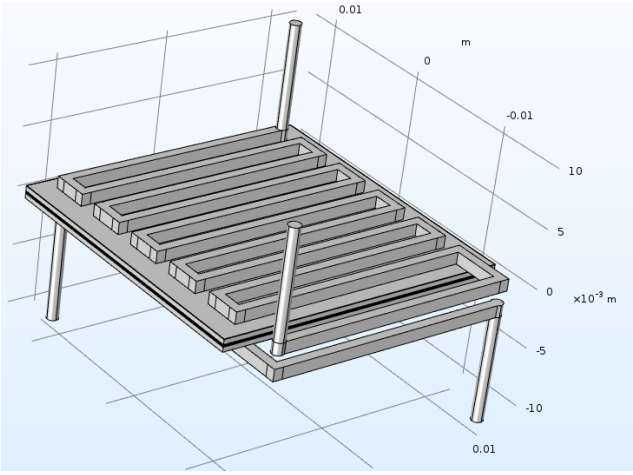

Figure 1. PEM fuel cell model

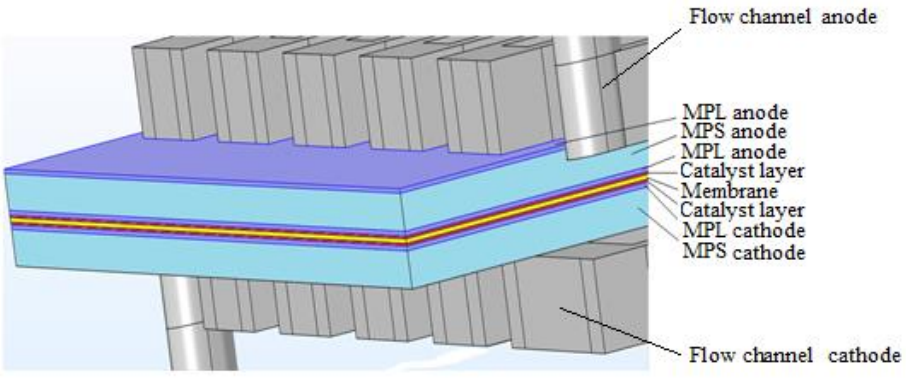

Figure 2. Details of the main layers and flow channels

Table 1. Geometrical parameters of the model

Parameter	Value (mm)
Flow channel length	21.2
Flow channel width	0.8
Flow channel height	1
Distance between channels	1.6
MPS thickness	0.406
MPL thickness	0.048
Catalyst layer thickness	0.03
Membrane thickness	0.0508

Table 2. Fuel cell model parameters used in this research

Parameter	Value	Reference
Membrane conductivity ∥	7.2 S/m	fuelcelletc.com
Membrane conductivity ⊥	5.05 S/m	fuelcelletc.com
Bipolar plate conductivity ∥	$1.11x10^{6}$ S/m	Schunk Ibérica
Bipolar plate conductivity ⊥	$5.26x10^{5}$ S/m	Schunk Ibérica
MPS electric conductivity	66667 S/m	http://zoltek.com/products/px30/
MPL electric conductivity	450 S/m	http://www.cabotcorp.com
Catalyst layer porosity	0.19208	Beruski (2017)
PTL porosity	0.63	fuelcelletc.com
MPS porosity	0.8	fuelcelletc.com
Reference exchange current density at anode	4175 A/m^2	Neyerlin et.al (2007)
Reference exchange current density at cathode	$2.55x10^{-10}$ A/m^2	Perez et.al (1998)
Cathodic Tafel slope	-65mV	
MPS permeability ∥	$1.3x10^{-11}$ m^2	Beruski (2017)
MPL permeability ⊥	$1.85x10^{-12}$ m^2	Beruski (2017)
Flow rate anode	160cm^3/min	Lopes et al. (2014)
Flow rate cathode	500cm^3/min	Lopes et al. (2014)
Operating pressure	206.84 kPa	Lopes et al. (2014)
Cell temperature	80°C	Lopes et al. (2014)

4. RESULTS AND DISCUSSIONS

In this present work, experimental data are compared with the modeling results for a single PEM fuel cell, operating at 80 ºC with flow rate in the anode and the cathode of 160 cm^3/min and 500 cm^3/min respectively. The initial simulation corresponds to the parameters indicated by tables 1 and 2, and the results are shown in Fig. 3 and Fig.4.

4.1 Effect of the specific surface area of the catalyst layer

The specific surface of a porous material is defined as the interstitial surface area of the voids and pores either per unit mass and this corresponds to the porosity measure in porous solids materials. High surface areas of active catalyst per geometric area of electrode are desirable to maximize PEFC performance. Was investigate the effect of the electrochemical active area of the catalyst over the fuel cell validation of the numerical model, we have varied this parameter between 700, 800 and 1000 cm^2/mg. Was also changed the cathodic Tafel slope and exchange current density at cathode to -76mV and $1.89x10^{-8}$ A/cm^2 respectively, since as, with the original table 1 values, very high values of specific surface area were required to validation of the numerical model. A good agreement between the experimental

and the results of the CFD were obtained for values of specific surface area to 700 cm^2/mg. The importance of simulating the specific surface area of the catalyst layer is to know for example, the degradation process during the operation of fuel cell. According the Carcadea et al. (2018) to investigate further the effect of the electrochemical active area of the catalyst over the fuel cell performance, the authors varied this parameter between 370 cm^2/mg to 870 cm^2/mg, and it is observed that there is an overall 22% increase in current density as the electrochemical active area is growing.

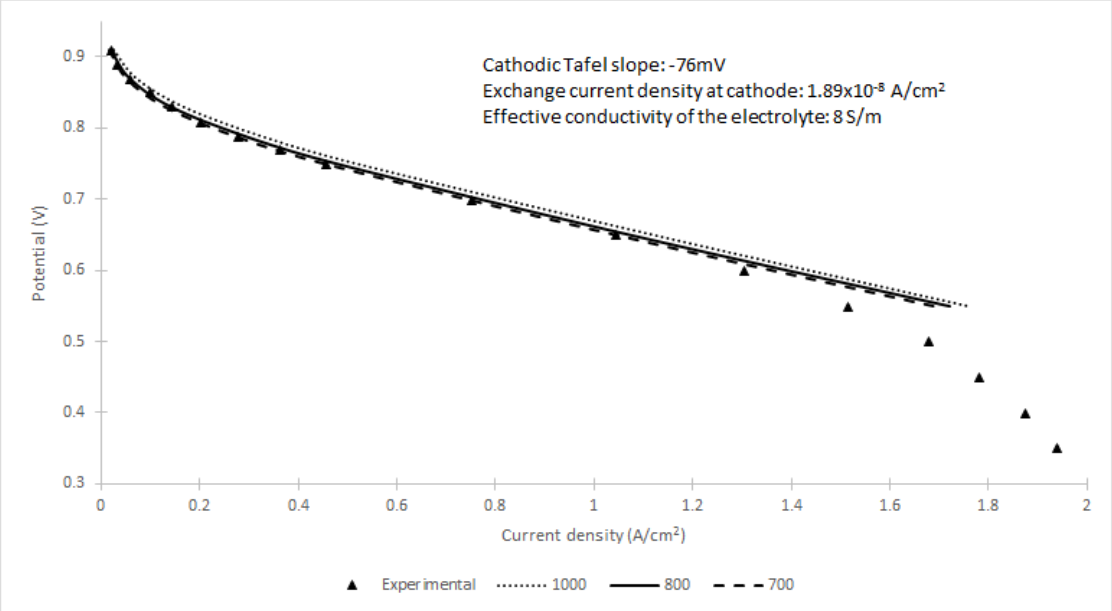

Figure 3. Comparison of experimental polarization data with numerical results having different specific surface area of the catalyst layer

4.2 Effect of the effective conductivity of the electrolyte

In the PEMFC the proton conductivity of the membrane is particularly important since it plays a significant role in controlling the performance of the fuel cell. The conductivity of Nafion membrane materials is complex, being dependent by a high level of hydration, the operating temperature, and thickness. Fig. 4 shows the impact of the effective conductivity of the electrolyte on the fuel cell performance. The models predict the performance curves for three different conductivity of the electrolyte values such as 4, 5, and 8 S/m (EC4, EC5 and EC8 respectively). As seen from the figure, the three curves have a similar behavior in the activation polarization, but, in the region by resistance polarization, begins to have a significant distance because of the conductivity difference and this affects the resistance of the electrolyte.

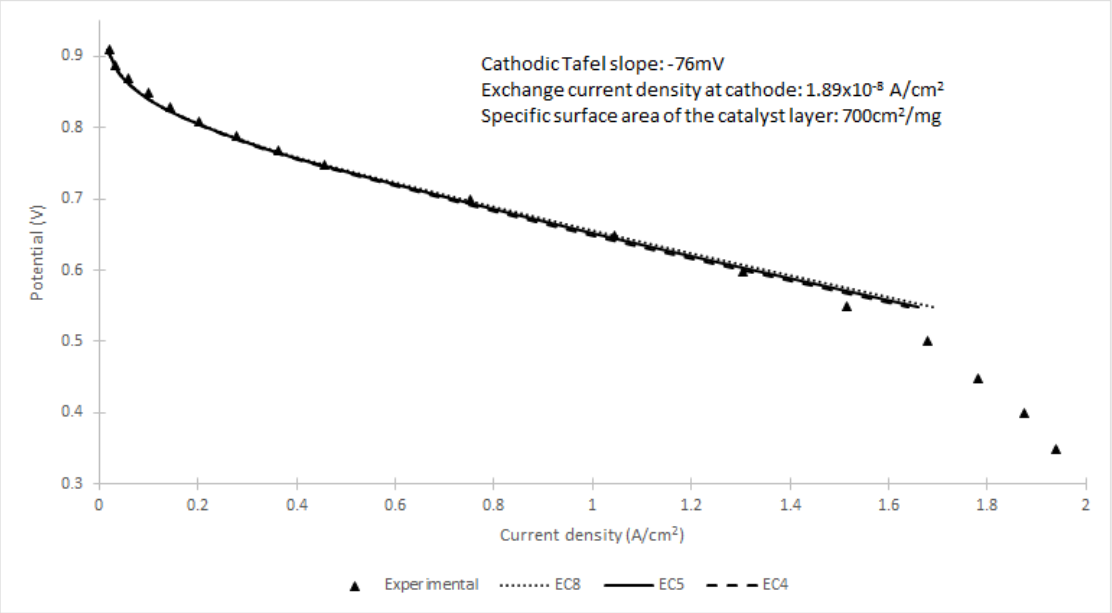

Figure 4. Comparison of experimental polarization data with numerical results having different electrolyte conductivities

5. CONCLUSIONS

Simulation using computational fluid dynamics is an important tool for analyzing differences between the main parameters. The following conclusions can be drawn from the results:

- Changing the specific surface area, it is possible to have a good approximation of the experimental polarization curve. This is totally related to the value of the generated current density.
- A good agreement between the experimental and the results of the CFD were obtained for values of specific surface area to 700 cm^2/mg;
- Membrane proton conductivity is an important parameter in the drop in ohmic resistance;
- The best conductivity values were between 4 and 5 S/m.

6. ACKNOWLEDEGEMENTS

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