EXPERIMENTAL AND NUMERICAL INVESTIGATON OF A PEM FUEL CELL. SINGLE CELL AND STACK ANALYSIS

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ABSTRACT

The present paper describes the work being done by INTA and University of Seville – AICIA in the framework of a joint research project in the field of Proton Exchange Membrane Fuel Cells (PEMFC). The main objective of the project is to develop a novel methodology for the characterization and investigation of fuel cell stacks, that combines experimental and Computational Fluid Dynamics (CFD) analysis. A CFD model based on the PEMFC Module implemented in FLUENT software is being developed for a single cell, and the polarization curve obtained is being validated against experimental results obtained at INTA facilities. At a second stage of the investigation, a method for the extrapolation of CFD single cell results to the complete stack is developed. The extrapolation method is being validated against experimental results obtained for the fuel cell stack with different numbers of cells. This paper describes the results of the early stages of the investigation and presents the methodology developed for the project. The developed model would allow researchers to use CFD for the complete fuel cell stack with reasonable computing facilities.

KEYWORDS

Fuel Cell, Simulation Tool, Stack, Computational Fluid Dynamics.

1. INTRODUCTION

PEM Fuel Cell models currently being applied and developed by designers and researchers can be considered as multi-dimensional and one-dimensional models [1]. Multi-dimensional models are based on CFD to solve governing equations, and provide high resolution results of flow characteristics of reactants, by-products, and charge transport. This is particularly advantageous for the analysis of a single cell given the detailed information that is provided by the model, but is limited for a stack because of the enormous computational time that would be required. These models are therefore applied to investigate parts of complex domains such as flow fields of a single cell and to predict the performance of a single cell.

By contrast, one-dimensional models are macroscopic models that describe layers in a cell. These simplified models do not provide detailed analytical mechanisms of a cell, but allow representations of a multi-cell stack, and therefore these models are preferred for investigating the complete system. However, as models are based on a one-dimensional approach, results must be considered with care as they may involve an important lack of accuracy.

The main objective of the research work presented in this paper is to develop a novel method for the characterization and investigation of fuel cell stacks. The method is based on both experimental and Computational Fluid Dynamics analysis. The strategy to accomplish this work is being presented in this paper. It must be noticed that this

paper describes the results of the early stages of the investigation, and mainly presents the methodology developed for the project.

2. RESEARCH STRATEGY AND METHODOLOGY

The model being developed is aimed to the analysis of any type of PEMFC, and for the initial development and validation the work is being performed on two different stacks. The stacks and cells being modelled correspond to commercially available models from ElectroChem Inc. Each stack consists of seven MEAs (Membrane Electrode Assembly) with Nafion-117 membranes. The MEAs are manufactured based on CCM (Catalyst Coated Membrane) technology. The main technical specifications are detailed in Table 1.

Table 1

Technical specifications of the fuel cell stack from ElectroChem Inc.

Specifications	
Average cell Voltage	0.65 +/- 0.05 V
Current Density	350 +/- 50 mA cm^{-2}
Total Power	180-280 mW cm^{-2}
Nominal power output	50 W
Dimensions	13.5 x 13.5cm x 13.5 cm
Net weight	4 kg
Electrode Assembly	50 cm^2, 7 MEAs
Type	Solid Polymer Electrode

A CFD model based on the PEMFC Module from FLUENT software is being developed for a single cell of each stack. The polarization curves for the single cells are obtained by running several simulations with different boundary conditions. The current

intensity-voltage curves obtained are being validated against experimental results obtained at INTA facilities, thus allowing for a detailed comparison between numerical and experimental results.

Secondly, an extrapolation method is being developed for the extrapolation of CFD single cell results to the complete stack. This would allow researchers to predict the complete fuel cell stack performance from CFD results of a single with cell, thus with reasonable computing facilities. In order to develop and validate the extrapolation method, experimental results are obtained for the fuel cell stacks with different numbers of cells. The results are expected to allow for the development of an accurate method for the extrapolation of CFD single cell results to the complete stack.

3. STACK MODEL DEVELOPMENT

The different research milestones to be accomplished during the research work are described in the following sections.

3.1. Single cell model development and calculation

3.1.1. Model description

A CFD steady state model for a single cell based on the PEMFC Module from FLUENT software is being developed. The model is solving not only the reactant gases flow and diffusion, but also the electrochemistry and current continuity, the liquid water generation and water transport, the membrane humidification, electric losses, heat transfer and other relevant phenomena. The equations used in the model are described in

[2]. The PEMFC model is based on the correlations proposed by Springer et al. [3], developed for Nafion-117 membranes.

3.1.2. Geometry and material properties

The geometry of the Bipolar Plates has been obtained from ElectroChem Inc., and the physical properties necessary for the model have been obtained from ElectroChem Inc., DuPont Technical Data Sheets (for Nafion-117), SGL Group (GDL provider) and from the literature [4,5,6,7]. A summary is listed in Table 2. There are still unknown values that will have to be obtained from the literature or experimentally. In a first approach, two different Bipolar Plates geometries are being analysed: a straight flow and a serpentine flow pattern, as shown in Figure 1.

Table 2

Physical Properties of the fuel cell materials.

Data	Units	Value	Source
Material Properties			
Bipolar Plate			
Material: Isotropic graphite			ElectroChem
Density	kg m^{-3}	1990	ElectroChem
Specific Heat Capacity	J $kg^{-1}K^{-1}$	710	[4]
Thermal Conductivity	W $m^{-1}K^{-1}$	120	ElectroChem
Electric Conductivity	ohm m	1.08E-05	ElectroChem
Gas Diffusion Layer			
Density	kg m^{-3}	320	SGL Group
Specific Heat Capacity	J $kg^{-1}K^{-1}$	*	
Thermal Conductivity	W $m^{-1}K^{-1}$	0.3	[5,7]
Electric Conductivity	ohm cm^2	0.015	SGL Group

Porosity	-	0.82	SGL Group
Viscous Resistance	m^{-2}	1.0E+09	[5]
Contact Angle	deg	*	
Thickness	mm	0.42	SGL Group
Catalytic Layer			
Density	kg m^{-3}	*	
Specific Heat Capacity	J $kg^{-1}K^{-1}$	*	
Thermal Conductivity	W $m^{-1}K^{-1}$	*	
Electric Conductivity	ohm m	*	
Porosity	-	*	
Viscous Resistance	m^{-2}	*	
Surface-to-Volume ratio	m^{-1}	*	
Contact Angle	deg	*	
Thickness	mm	*	
Membrane			
Density	kg m^{-3}	1980	DuPont
Specific Heat Capacity	J $kg^{-1}K^{-1}$	2000	
Thermal Conductivity	W $m^{-1}K^{-1}$	0.13	[7]
Electric Conductivity	ohm m	Model	[3]
Equivalent Weight	kg $kmol^{-1}$	1100	[6]
Thickness	mm	0.175	DuPont
PEM Model Parameters			
H2 Species Diffusivity	m^2 s^{-1}	3.0E-05	[4]
O2 Species Diffusivity	m^2 s^{-1}	6.0E-05	[4]
H2O Species Diffusivity	m^2 s^{-1}	3.0E-05	[4]
Pore Blockage Saturation Exponent	-	*	

* denotes unknown values.

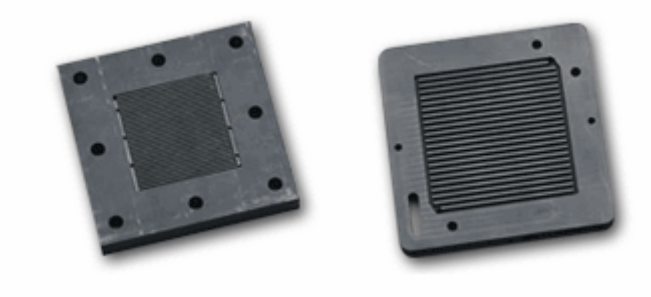

Figure 1: Geometry of the Bipolar Plates: serpentine flow pattern (left), straight channel flow pattern (right).

3.1.3. Mesh generation

Previously to the work presented in this paper, a different cell with a different MEA and Bipolar Plate have been studied. The MEA was a Celtec®-P1000 from BASF-PEMEAS, which is based on high temperature polymer polybenzimidazole (PBI) and phosphoric acid for a high temperature operation (120ºC-180ºC). However, the models of the FLUENT PEMFC Module are based on correlations derived for Nafion-117 membranes [2,3], and therefore the software cannot be directly applied to the resolution of cells with PBI membranes. However, the simulations performed with this cell were used to assess the meshing requirements needed for successful CFD simulations of fuel cells.

A mesh sensitivity study has been performed in order to ensure that CFD results are independent from mesh spatial discretization. The procedure applied to accomplish this has been performed by following standard CFD Best Practice Guidelines [8]. The pressure drop of the flow along the channels was selected as monitoring variable. The geometry of the Bipolar Plate consisted of a triple serpentine flow pattern as shown in Figure 2, with an active surface area of 45 cm^2. Channel width and depth, and rib width

is 0.764 mm. The description of the meshes generated for the study is presented in Table 3, and results obtained are presented in Figures 3 to 5.

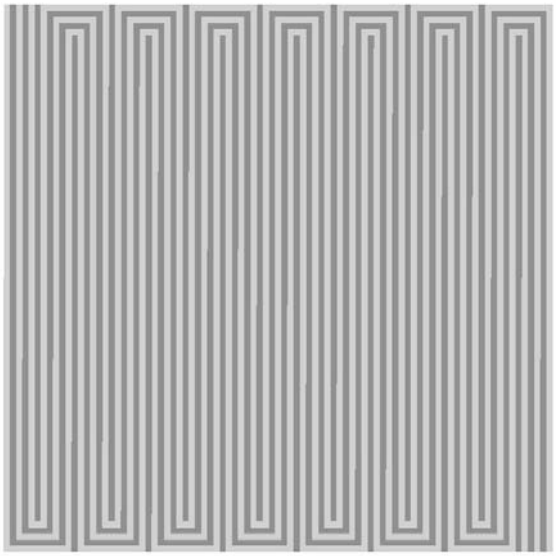

Figure 2: Geometry of the Bipolar Plate used for the mesh discretization study.

Table 3

Description of the meshes used for the mesh sensitivity study.

Mesh ID	Ne (x1E3)	Nn (x1E3)	Ne (d channel)	Ne (w channel)	Ne (L channel)	Ne t GDL
Mesh 1	420	490	5	5	40	4
Mesh 2	875	980	7	7	40	5
Mesh 3	1925	2125	10	10	60	5

Ne – Number of elements.
Nn – Number of nodes.
d channel – Channel depth.
w channel – Channel width.
L channel – Channel length.
t GDL – Gas Diffusion Layer thickness.

From the results obtained in this study, a Fuel Cell Meshing Best Practice Guidelines procedure has been developed with the following conclusions, applicable to cells of dimensions similar to the cell studied:

1. The channel cross-section must be resolved with at least 7x7 elements.
2. The channel length must be resolved with at least 40 elements. If non-conformal meshes are to be used due to a cross-flow bipolar plate configuration, the minimum number of elements must be 80.
3. The thickness of the different layers of the MEA: gas diffusion layers, catalytic layers and membrane, must be resolved with at least 5 elements.

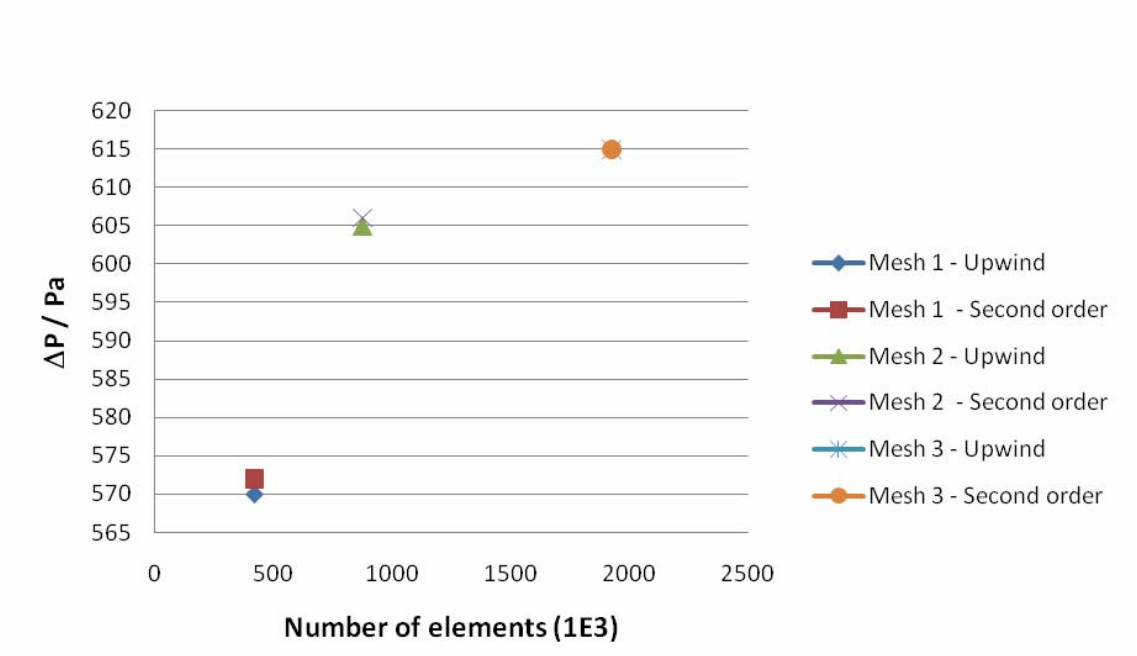

Figure 3: Mesh study results. Channel pressure drop versus number of mesh elements.

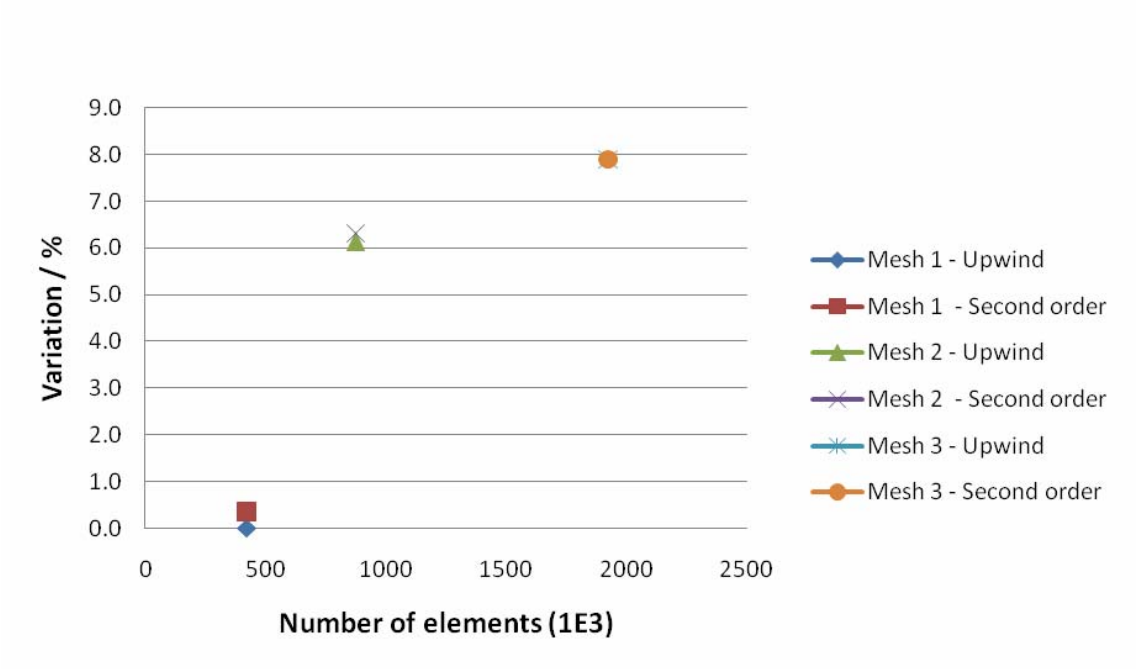

Figure 4: Mesh study results. Relative variation of the results related to mesh 1 results (coarsest).

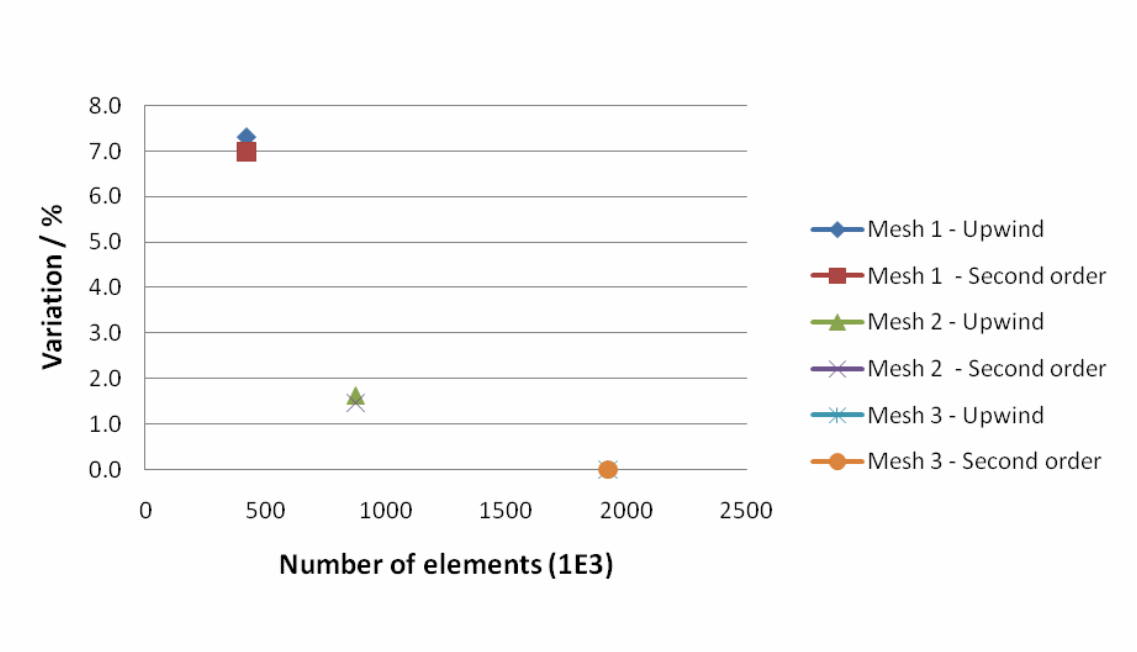

Figure 5: Mesh study results. Relative variation of the results related to mesh 3 results (finest).

The conclusions listed above can be considered as a general rule for the meshing requirements of a cell. Further mesh refinement would be required for a definite analysis, but the mesh size must be limited to a practical extension so that the model can be generally applied. The finest mesh run with this model required 3.0 GB RAM, so it has been decided not to further refine the mesh.

3.1.4. Calculation procedure and results

The polarization curve of the cell is the main result of the single cell analysis needed for the model being developed. This is obtained by running a set of simulations with different boundary conditions either for the cell voltage or the cell current intensity. The simulations of the cells have not been performed yet. However, results for the Celtec®-P1000 cell are presented in Figure 6 in order to show a typical I-V curve obtained from the simulations. As described in the previous section, the results obtained for this cell are not correct and do not match the characteristic curve provided by the manufacturer, as PBI membranes are not directly solved by the software.

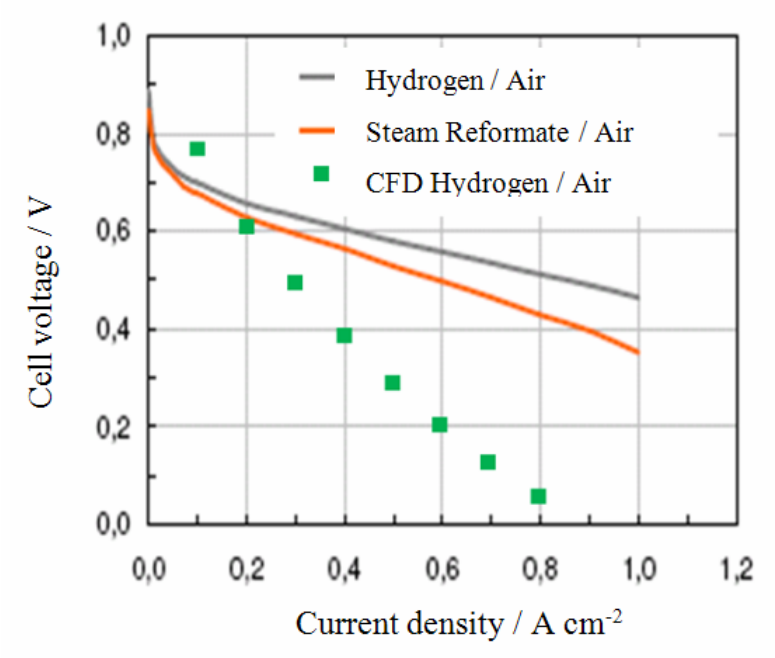

Figure 6: Current intensity - Voltage curve: results from the CFD calculation for the Celtec®-P1000 cell.

The simulations will be performed for both cells (straight flow pattern and serpentine flow pattern) and a set of I-V curves will be obtained for each cell, setting different reactants mass flows as boundary conditions. Both geometry and mesh generation will be parameterized in a script file, together with the CFD runs, in order to allow for a quick analysis of the influence of different fuel cell geometrical designs, operating conditions or material properties, in the single fuel cell and stack performance.

3.2. Single cell model validation

The current intensity-voltage curves obtained for the fuel cells (straight flow pattern and serpentine flow pattern) will be validated against experimental results obtained at INTA facilities, thus allowing for a detailed comparison between numerical and experimental results.

3.3. Extrapolation method development

An extrapolation method will be developed for the extrapolation of CFD single cell results to the complete stack. This would allow researchers to analyse the stack performance from single cell CFD results, thus with reasonable computing facilities.

The model being developed must consider the fact that each cell of the stack may process a different mass flow of reactants [9]. This depends on the stack manifold geometry, the number of cells in the stack, the total mass flow and the pressure drop of the flow through each cell [10,11,12]. Therefore, it is not possible to assume that the voltage of the stack is the voltage of a cell multiplied by the number of cells in the stack. The developed model is considering this effect, according to the following strategy:

First, I-V curves of a single cell for different reactants mass flow rates are needed as input parameters. The curves are being obtained by means of CFD calculations as described previously. Secondly, the reactant mass flow rates through each cell must be predicted. This can be obtained via CFD calculations of the stack manifolds or from a theoretical model based on hydraulic resistances, as in [11,12]. The second alternative is preferred as it will allow for a more general model, applicable to different manifold and stack geometries, and significantly more straightforward to use.

With the information obtained the I-V curve of the complete stack can be calculated by combining the predicted mass flow rate for each cell with the predicted I-V curve of the cell with this mass flow rate. Comprehensive sensibility analysis of the stack performance for different geometrical designs, operating conditions, or material properties, can be therefore performed.

3.4. Extrapolation method validation

In order to validate the extrapolation method developed, experimental results will be obtained at INTA facilities for the fuel cell stacks with different number of cells. The results may be used as well to adjust certain model constants, so the theoretical model would be then based on a semi-empirical approach as well.

4. CONCLUSIONS

A research methodology for the development of a novel method for the characterization and investigation of fuel cell stacks is presented, together with preliminary results. The method is based on experimental and Computational Fluid Dynamics analysis.

A CFD model based on the PEMFC Module from FLUENT software is being developed for a single cell. The polarization curve of the single cell is obtained by running several simulations with different boundary conditions. The current intensity-voltage curve obtained is being validated against experimental results obtained at INTA facilities, thus allowing for a detailed comparison between numerical and experimental results.

Secondly, an extrapolation method is being developed for the extrapolation of CFD single cell results to the complete stack. This would allow researchers to analyse the stack performance from single cell CFD results, thus with reasonable computing facilities. In order to develop and validate the extrapolation method, experimental results are obtained for the fuel cell stacks with different numbers of cells. The results are expected to allow for the development of an accurate method for the extrapolation of CFD single cell results to the complete stack.

5. ACKNOWLEDGMENTS

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