PROJECT DESCRIPTION

Title: "MODELING, SIMULATION AND EXPERIMENTAL VALIDATION OF POLYMER ELECTROLYTE MEMBRANE FUEL CELLS AND ALKALINE MEMBRANE FUEL CELLS"

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1. BACKGROUND

The continuous growth of the global energy demand and vehicle utilization around the world is requiring the development of fuel alternatives. In that context, fuel cells are one of the most efficient and cleanest alternatives to generate electricity. Fuel cell technology has advanced considerably in recent years, with the development and testing of stationary power generation and vehicular applications [1-4]. The main reason why fuel cells are not used extensively is that, economically, they are not competitive yet. One way of reducing cost is to develop lower cost components that could bear higher operating temperatures and allow for higher power density. A more general alternative is the optimization of the flow geometry subject to global constraints (e.g., fixed volume), with the objective of maximizing total power or power density. This approach is general because it could be used together with other enhancement methods, e.g., new materials, and new hydrogen separation from natural gas techniques inside the fuel cell (internal reforming).

Many fuel cell models have been published in the technical literature. For example, there are analytical [5] and numerical models [6-8] that assume a bi-dimensional geometry, steady state operation, uniform temperature distribution throughout the fuel cell compartments, and with different oxidant and fuel pressures. Zhou and Liu [9] presented a steady state tri-dimensional model for polymer electrolyte membrane fuel cells, PEMFC. Those bi- and tri-dimensional models are not appropriate for the flow geometry optimization because they would require the solution of a system of complex partial differential equations to test a large number of different flow configurations. No similar model to the ones developed by this proposal's research team was found in the literature, such that the single fuel cell and/or stack pressure and temperature internal gradients, gas channel pressure drops and their effect on cell performance are accounted for simultaneously or in isolation.

In this project, the methodology divides the single cell in several control volumes, as shown in Fig. 1, which correspond to the most representative parts of the flow system. All flow phenomena that are present are taken into account. The model is described by a system of algebraic and ordinary differential equations whose solution consists of the history of temperatures and pressures in each control volume, and of the polarization and net power curves for the entire system. The model is simple enough to ensure low computational time to obtain the solution for each specific geometric configuration, such that it is possible to simulate the flows in a large number of flow configurations that are required by the optimization process.

The system architecture is subject to a fixed volume constraint, realistically recognizing the limited space availability in any engineering project. There are several degrees of freedom in the fuel cell configuration, i.e., the thicknesses of the two gas channels (fuel and oxidant), two diffusive layers, two reactive layers (anode and cathode), and the alkaline membrane (electrolyte). The single cell also interacts with the adjacent cells in a stack (set of single cells), and/or the ambient. To determine the single cell net power, a balance between the total electric power produced and the required pumping power to feed the cell with fuel and oxidant through the micro-channels was performed. Therefore, a software was made available to the scientific and industrial communities as a design, control and optimization tool for the development and improvement of single alkaline and polymer electrolyte membrane fuel cells.

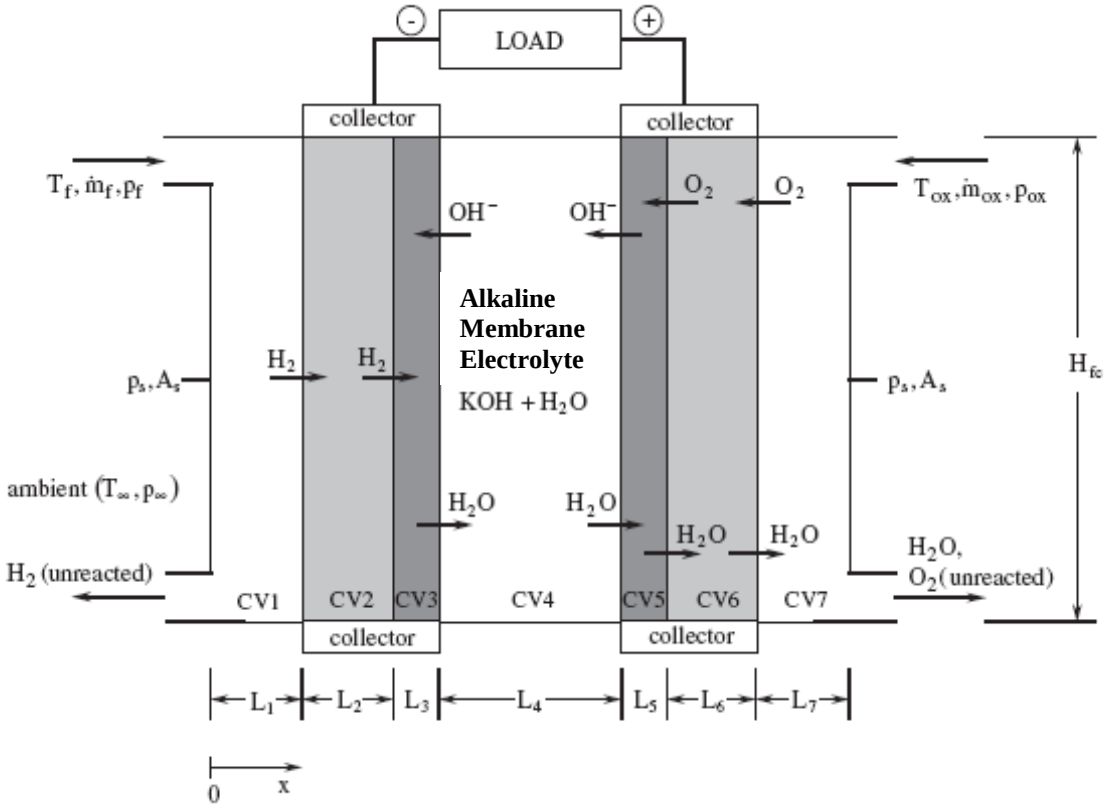

Figure 1 – Division in control volumes of a single alkaline membrane fuel cell: CV1 – fuel gas channel (H_2); CV2 – anode diffusive layer; CV3 – anode reactive layer; CV4 – alkaline membrane electrolyte; CV5 – cathode reactive layer; CV6 – cathode diffusive layer, and CV7 – oxidant gas channel (O_2).

The main conclusion was that the thermodynamic optimization procedure ("constructal design") [10] needed to be extended to the fuel cell stack level, to optimize the thermal and water management, the geometric configuration of the micro-channels, and the structural assembling of the single cells in a stack for maximum net power density and/or efficiency. In general, the geometric flow configuration must be designed to minimize pressure drop (i.e., reducing pumping power) at the same time that provides adequate and uniformly distributed mass transfer through the diffusive layers to the catalyst surface in the electrodes for the reactions to occur.

The study of PEMFC allowed for understanding fuel cell components and operation. Those cells use mainly nafion (the acid polymeric membrane produced by Dupont, USA) as the electrolyte, and require significant platinum content in the electrodes, as the catalyst. Nickel, for example, has a catalytic potential similar to platinum. Although much cheaper than platinum, nickel cannot be used as catalyst in PEMFC electrodes, due to the acid medium (nickel is not compatible with an acid medium). Platinum is a precious material, and therefore one of the reasons for PEMFC high cost. Therefore there are two important reasons to focus the research on developing alkaline membrane fuel cells: i) with respect to current alkaline fuel cells, the herein proposed alkaline membrane fuel cell has the advantage of a membrane instead of a liquid electrolyte, and does not require elaborated seals to operate, and ii) with respect to polymer electrolyte membrane fuel cells, platinum-free electrodes could be used, since cheaper materials such as nickel, iron and/or cobalt could be used as catalysts in an alkaline medium, which would significantly lower fuel cell cost and allow the use of materials that are abundant in nature instead of platinum that is expensive and has known limited reserves worldwide.

This cell works at low temperatures, but requires oxygen as the oxidant, and not simply air as the PEMFC, since it is easily susceptible to carbon dioxide poisoning. However, the cell is expected to allow for a good performance with platinum free electrodes (nickel is compatible with an alkaline medium). Additionally, the experiments showed that the electrolyte could be a cellulosis based membrane, with a low cost. As a result, this proposal's research team understands that an optimized alkaline membrane fuel cell project could be very competitive with the PEMFC.

The maturation of the team's knowledge on the subject allowed for the development in the laboratory of an AMFC prototype using a cellulosis based membrane and platinum-carbon electrodes, as it is shown in Fig. 2.

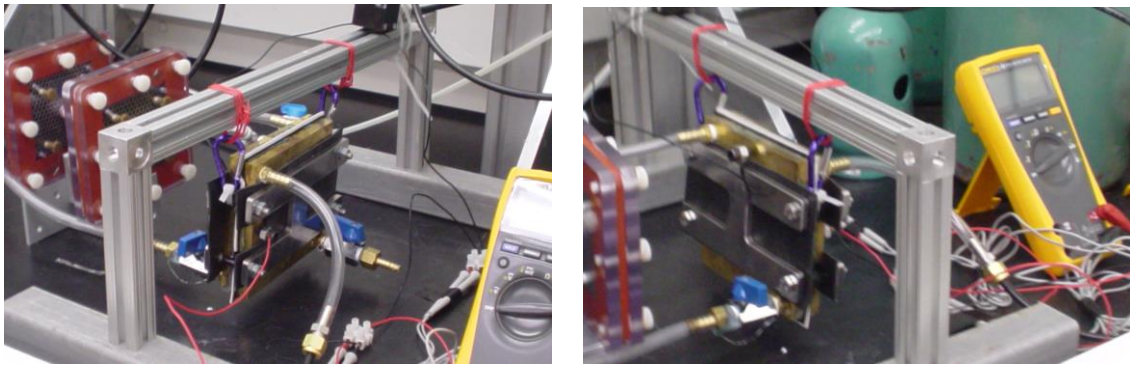

Figure 2 – Prototype of an alkaline membrane fuel cell (AMFC) made with a cellulosis electrolyte.

2. OBJECTIVES AND ACTIVITIES

2.1. Objectives:

The project is structured as a sequence of theoretical, numerical and experimental activities to accomplish the mathematical modeling and the development of polymer electrolyte membrane fuel cells and alkaline membrane fuel cells optimization tool. Finally, it is intended that the project will contribute to create new low temperature fuel cell alternative technology to PEMFC technology.

The main objective is to develop a new alternative fuel cell type and demonstrate a methodology based on the physical laws to optimize thermodynamically fuel cell packages for maximum performance.

2.2. Activities:

The project is divided in several activities (phases) to be pursued sequentially and/or in parallel:

1. Mathematical thermodynamic modeling of a unit PEM fuel cell, to predict performance as a function of geometric and operating parameters;
2. Chemical, thermal and morphologic characterization of membrane electrolyte assembly;
3. Experimental validation of numerical results and parameters adjustment of the mathematical model for selected cases;
4. Mathematical modeling of a single alkaline membrane fuel cell (AMFC), to predict performance as a function of operating and geometric parameters, for optimization;
5. Development of a prototype of a single alkaline membrane fuel cell (AMFC);
6. Experimental validation of numerical results and parameter adjustment of the mathematical model;
7. Checking for robustness of the results found comparing AMFC results for different alkaline solution concentrations.

3. METHODOLOGY

3.1. Mathematical thermodynamic modeling of a unit polymer electrolyte membrane fuel cell (PEMFC), to predict performance as a function geometric and operating parameters.

The main features of a hydrogen polymer electrolyte membrane fuel cell (H_2 PEMFC) are shown in Fig. 3. The fuel may be pure hydrogen, or a diluted hydrogen mixture generated from a hydrocarbon reformation process. For simplicity, the model is based on the assumption that the fuel stream is pure hydrogen, and that the oxidant is pure oxygen.

The fuel cell is divided into seven control volumes that interact energetically with one another. The fuel cell also interacts with adjacent fuel cells in a package, and/or with the ambient. Additionally, two bipolar plates (interconnects) are presented: these have the function of allowing the electrons produced by the electrochemical oxidation reaction at the anode to flow to the external circuit or to an adjacent cell. The control volumes (CV) are the fuel channel (CV1), the anode diffusion backing layer (CV2), the anode reaction layer (CV3), the polymer electrolyte membrane (CV4), the cathode reaction layer (CV5), the cathode diffusion backing layer (CV6) and the oxidant channel (CV7).

The model consists of the conservation equations for each control volume, and the equations accounting for electrochemical reactions, where reactions are present. The reversible electrical potential and power of the fuel cell are then computed (based on the reactions) as functions of the temperature and pressure fields determined by the model. The actual electrical potential and power of the fuel cell are obtained by subtracting from the reversible potential the losses due to surface overpotentials (poor electrocatalysis), slow diffusion and all internal ohmic losses through the cell (resistance of individual cell components, including electrolyte membrane, bipolar plates, interconnects and any other cell components through which electrons flow). These are functions of the total cell current (I), which is directly related to the external load (or the cell voltage). In sum, the total cell current is considered an independent variable in this study.

3.2. Experimental validation of numerical results and parameters adjustment of the mathematical model

In this phase, the numerical results obtained after the computational implementation of the mathematical model of item 3.1 for a unit fuel cell was validated and adjusted experimentally considering the properties measured during the characterization step. This is a vital intermediate stage of the study, before the system optimization, since it will allow the evaluation of the accuracy of the numerical results obtained with the mathematical model.

3.4. Mathematical modeling of a single alkaline membrane fuel cell (AMFC), to predict performance as a function of operating and geometric parameters

In this phase, the mathematical model for a liquid electrolyte alkaline fuel cell was adapted to the new alkaline membrane fuel cell (the AMFC schematically shown in Fig. 1).

3.5. Prototype of a single alkaline membrane fuel cell (AMFC)

This phase consisted of the improvement in the laboratory of a prototype of the single alkaline membrane fuel cell, which uses a cellulosis based membrane electrolyte and platinum-carbon electrolytes that was recently developed by this proposal's research team, as shown in Fig. 2. The work had the objective of testing alternative compositions of the alkaline membrane, as well as the improvement of the other internal components, as follows: i) project of interconnecting plates, including selection of materials, and micro-channels design for the transport of fuel and oxidant for minimum pressure drop and maximum uniform distribution [11], and ii) project, selection of materials.

3.6. Experimental validation of numerical results and parameter adjustment of the mathematical model

The mathematical model adjustment is an important step that will allow for the improvement in the formulation to better capture the physical phenomena involved in the process. This was an iterative process, converging when the numerical results approach the experimental measurements within a narrow and pre-specified

error margin. This is an intermediate and vital stage of the study, before the system optimization, since it will allow for the evaluation of the accuracy of the numerical results obtained with the mathematical model.

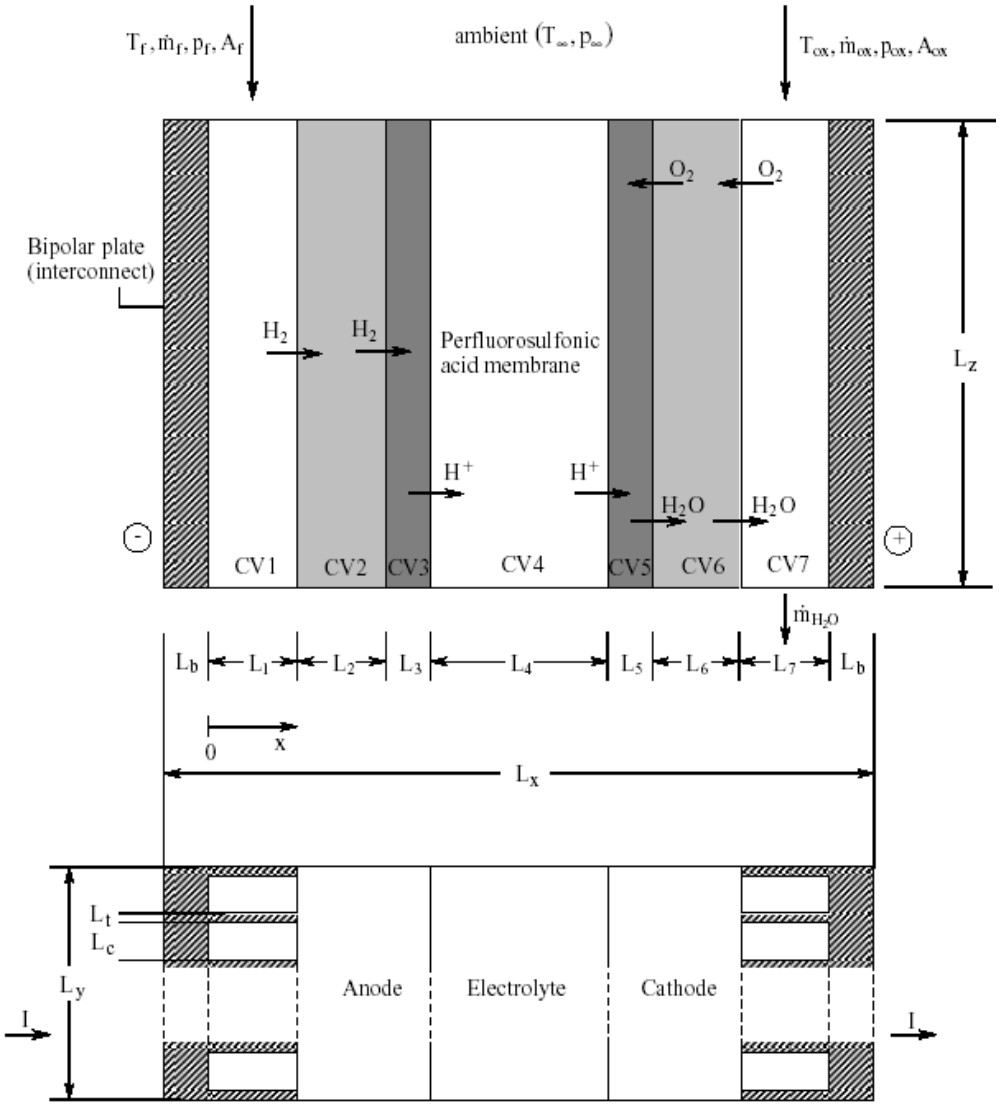

Figure 3 – Model of hydrogen-oxygen unit fuel cell.

The procedure consisted of the utilization of the alkaline membrane fuel cell built in the laboratory and the recording of measurable physical quantities (e.g., temperature, pressure, current density, voltage, power density) for selected cases. Uncertainties were computed and the experimental measurements compared to the corresponding numerically calculated variables. The model parameters were adjusted appropriately, if necessary, by the solution of the inverse problem of parameter estimation [12]. In order to test the robustness of the model we performed experiments for different electrolyte concentration and checked if the numerical results matched with the experimental results.

4. RESULTS AND IMPACTS

Results and/or expected products

1. Production of a comprehensive and simplified PEMFC mathematical model;

2. Production of a comprehensive and simplified AMFC mathematical model;
3. Production of two prototypes: i) single AMFC;
4. Production of an experimentally tested software for design and optimization of AMFC to be utilized by the industry and academia.

5. MECHANISMS OF EXECUTION MANAGEMENT

The research team is composed by professors of two universities, i.e., Florida State University, FSU, and Federal University of Parana, UFPR (advisor and co-advisor) and the PhD student, all names mentioned at the beginning of this document. This scientific collaboration between both universities has been established since 1998, resulting in several joint archival publications and projects, and currently has an ongoing international project funded by the Air Force Office of Scientific Research, AFOSR, on solid oxide regenerative fuel cells [13].

The project is multidisciplinary and the objectives were intended to be accomplished by the complementary technical competences of the involved technical teams. In order to execute the project a series of articulations were established between the researchers involved in this collaboration. Therefore, it was a cooperative initiative that intends to establish a research team in an area of the NSF interest.

The predicted articulations will occur through the following mechanisms:

Information system: the internet is intended to be used as a constant communication and information diffusion mean among the project members. The e-mail was employed as the main integration mean between the members of the team.

Technical meetings: monthly technical meetings were held and the decisions and information exchanged between the principal investigator and team members with the objective of planning and synchronizing the activities, discussing the problems and directions of the project.

Seminars and workshops: annually, seminars were organized at Florida State University, where the participants presented the evolution of the work and the achieved results.

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