CFD BASED PROTON EXCHANGE MEMBRANCE FUEL CELLS MODEL

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Abstract

At the beginning of the 21st century, fuel cells appear poised to meet the power needs of variety of applications. Fuel cell systems are available to meet the needs of applications ranging from portable electronics to utility power plants. In addition to the fuel cell stack itself, a fuel cell system includes a fuel processor and subsystems to manage air, water, thermal energy, and power. The overall system is efficient at full and part-load, scaleable to a wide range of sizes, environmentally friendly, and potentially competitive with conventional technology in first cost. Promising applications for fuel cells include portable power, transportation, building cogeneration, and distributed power for utilities. For portable power, a fuel cell coupled with a fuel container can offer a higher energy storage density and more convenience than conventional battery systems. With the development of improved membranes, catalysts and bipolar plates, Proton Exchange Membrane (PEM) fuel cells will play an important role in the near future as a new power source. The design and control of the fuel cells may be advanced by Computational Fluid Dynamics (CFD) techniques. CFD has been used to generate three-dimensional models of PEM fuel cells with the purpose of understanding the physics inside the fuel cells and improving the fuel cell performance. The performance of the fuel cell can be affected significantly by the heat generated inside its Proton Exchange Membrane (PEM). Further, water evaporation and condensation generated by temperature change inside fuel cell control humidity of the membrane and vary the local current density value and all of these phenomena need to be included in the models.

In this paper, we provide an overview of the numerical and modelling ingredients required for the successful application of CFD. The application of CFD to Fuel Cells is discussed and some of the challenges highlighted. The fluid flow and transport phenomena in a fuel cell are quite complex due to the coupling of convective heat and mass transport with phase change, porous media and electrochemistry. Progress made in three-dimensional computational modelling of these transport phenomena is presented.

Keywords—fuel cell, PEMFC, thermal & water management, flow field, modelling, simulation.

I. INTRODUCTION

Fuels cells use continuous transformation of chemical energy into electrical power without thermal-to-mechanical conversion. In recent years, the interest in development of fuel cell systems has accelerated. The Proton Exchange Membrane fuel cell operates at low temperature and higher energy density and less polluting energy conversion promise of these devices make them feasible for use in stationary, portable and automotive applications. In particular, for automotive and portable applications, the Proton Exchange Membrane Fuel Cells are considered as the most successful candidates for replacing current power generating devices. Their high energy efficiency potential, possibly up to 50-70 %, which is unlimited to Carnot cycle efficiency, very low greenhouse emissions, quieter and reliable operation because of none or limited number of moving parts and scalability allow them to replace Internal Combustion Engines for vehicle applications and batteries for portable devices.

II. PEMFC OVERVIEW

Like any electrochemical device, A Proton Exchange Membrane (PEM) Fuel Cell system consists of an anode, a cathode and an electrolyte. A polymer membrane is used as the electrolyte in PEM Fuel Cell systems. Each one of the anode and cathode electrodes consist of gas channel, gas diffuser and catalyst layer, in which the electrochemical reactions take place as shown in Figure-1.

PEM fuel cells generate electric potential by separating the oxidation of hydrogen into two catalyzed steps performed on opposite sides of an electrolyte membrane [2]. The end products are water, water vapour, and heat. A 2D slice of a unit cell is shown in Figure-2

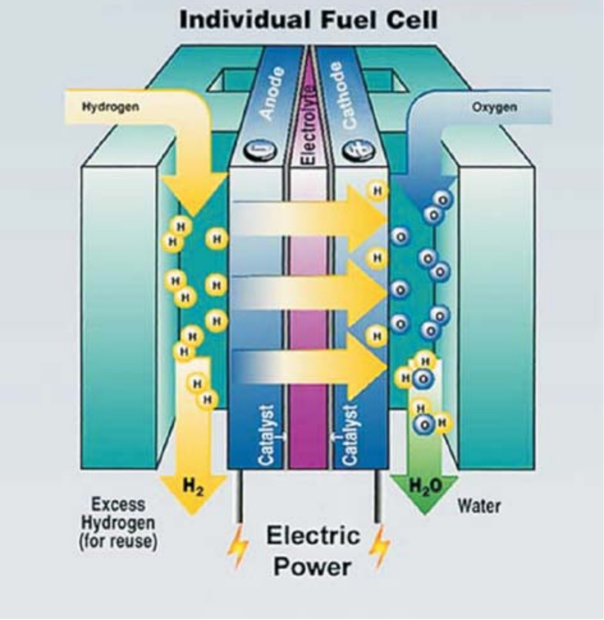

Fig. 1. Fuel Cell Stack

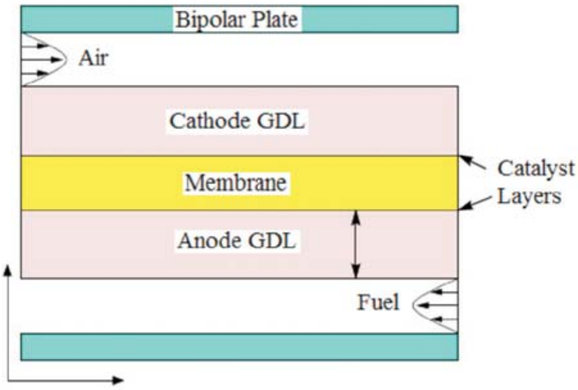

Fig. 2. The model geometry for a fuel cell

III. CFD OVERVIEW

Computational Fluid Dynamics (CFD) is a design tool that has been developed over the past few decades and will be continually developed as the understanding of the physical and chemical phenomena underlying CFD theory improves. The goals of CFD are to be able to accurately predict fluid flow, heat transfer and chemical reactions in complex systems, which involve one or all of these phenomena. Presently, CFD is being increasingly employed by many industries either to reduce manufacturing design cycles or to provide an insight into existing technologies so that they may be analyzed and improved. As a design tool, CFD presently sits behind experimental analysis due to the fact that CFD does not produce absolute results. The reason for this is that the numerical methods, which govern the solutions in a CFD problem, rely on several modeling assumptions that may not have been validated to a satisfactory level. However, CFD presently offers itself as a powerful design tool and even more so in the future because:

- Dangerous or expensive trial and error experiments can be simulated and design parameters observed prior to any physical prototype being constructed.
- Computers are becoming even more powerful and less expensive, thus allowing larger CFD simulations to be calculated, or more detailed simulations of present CFD problems.
- The numerical schemes and physical models that are the building blocks of CFD are continually improving.
- If a CFD model can be established yielding accurate results on one particular design, then the model can be used as a tool of prediction for that design under many different operating conditions.

IV. CFD PROCEDURES

- The geometry of the problem is defined.
- The volume occupied by the fluid is divided in to discrete cells. The mesh may be uniform or non-uniform.
- The physically modeling is defined.
- Boundary conditions are defined. This involves specify the fluid, behavior and properties at the boundaries of the problem. For problems, the initial conditions are also defined.
- The simulation is started and the equations are solved iteratively as a steady state or transient.
- Finally a post processor is used for the analysis and visualization of the resulting solution.

V. COMPUTATIONAL FUEL CELL MODELING

A proper modeling of the transport process requires understanding of airflow direction, temperature differences and pressure drops through the design long before coming to fruition. These issues lead to intriguing mathematical phenomena at the limit of continuum mechanics, including degenerate free-boundary problems requiring novel computational methods [3]. The development of a predictive computational model of heat and water management requires an understanding of gas and water transport in bipolar plates, in turn demanding development of innovative numerical schemes to adapt to the widely disparate time and length scales present in the system as shown in Figure-3.

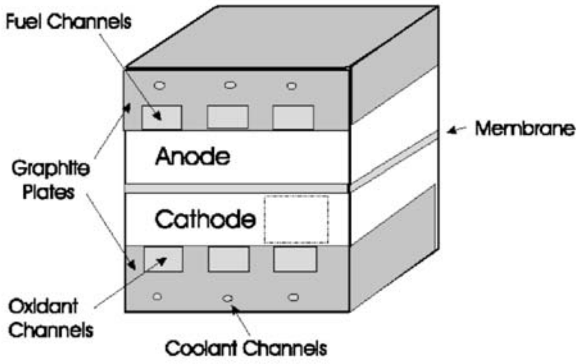

Fig. 3. The 3D Structure of Unit Cell

In the last few years, several large computational fluid dynamics (CFD) code vendors have become interested in developing comprehensive fuel cell computational models. Some examples are the modules developed by CFX , Gambit, Fluent , Matlab, etc. These CFD codes provide convenient 3D meshing and visualization tools and robust solvers for the traditional fluid dynamics elements of fuel cell models. These codes will provide a platform for validated models of elements unique to fuel cells to be integrated into the big picture. However, preliminary models suggest that the delicate balance of temperature, condensation and liquid water transport in the GDEs will be difficult to capture accurately in these general packages. Also, larger scale problems such as electrical coupling of cells in stacks and long time transients will have to be handled by specialized codes.

Collaboration between modeling and experimental work is needed in the development of models for fuel cells, as in other similar fields. Experimental work can serve first to guide and validate models and allow parameters to be fit [5]. In turn, models can identify critical parameters that be the subject of experimental measurement or the target for materials engineering. Some of the more important aspects of fuel cell modeling are listed below.

- Mass transport of species in membrane materials.
- Condensation and two phases flow models for gas diffusion layers.
- Capillary, hydrophobicity and rivulet modeling
- Unit cell modeling

VI. FLOW FIELD DESIGN

The flow field design of a Flow Field Plates heavily influences the performance of a PEMFC. It must uniformly distribute the reactant gases over the MEA and prevent product water flooding. If either of these functions are impaired the reactants will inefficiently be supplied across the MEA causing a loss in performance. Additionally, it must provide good electrical contact with the MEA to give low cell electrical resistance. There are three aspects to flow field design: (i) the distribution pattern, (ii) the cross section shape and (iii) the land and channel dimensions. [6], [7]. They are shown in Fig. 4.

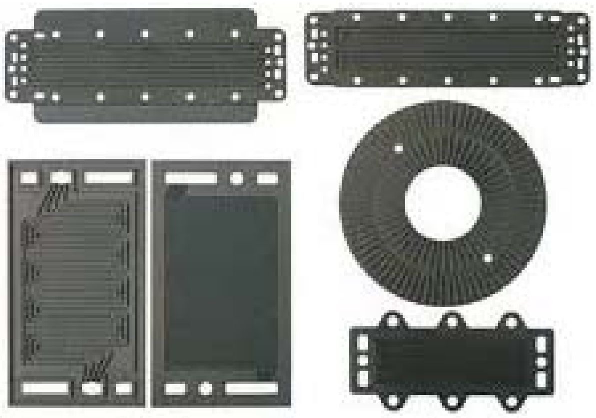

Fig. 4. Flow Field Plates

VII. CONCLUSION

1. Improving PEM fuel cell performance could not be satisfactory with only experimental studies.

2. One-dimensional models gave the principle thought of physics inside PEM fuel cells and fundamental for multidimensional simulations.
3. Two-dimensional models using computation fluid dynamics technique gave more realistic of PEM fuel cell simulation and enhance understating of PEM fuel cell however; this cannot achieve the development of flow-field design, comparison of predictions with experimental data.
4. Three-dimensional simulation using CFD approach presented the most realistic models and significantly comparable with experimental cells with variety of flow-field patterns. This will lead us to capture the actual operation of PEM fuel cell, such as transient response, water management, thermal management, pressure drop in stack, etc.
5. Future work will focus on building mathematical modelling using computer methods to solve fundamental equations of fluid flow.

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