V.F.1 Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization

J. Vernon Cole
CFD Research Corporation (CFDRC)
215 Wynn Drive, 5th Fl.
Huntsville, AL 35805
Phone: (256) 726-4852
E-mail: jvc@cfdrc.com

DOE Managers
HQ: Donna Ho
Phone: (202) 586-8000
E-mail: Donna.Ho@ee.doe.gov
GO: David Peterson
Phone: (720) 356-1747
E-mail: David.Peterson@go.doe.gov

Technical Advisor
Walt Podolski
Phone: (630) 252-7558
E-mail: podolski@anl.gov

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- Ballard Power Systems, Burnaby, BC, Canada
- BCS Fuel Cells, Bryan, TX
- ESI US R&D, Huntsville, AL
- Techverse, Cary, NC
- SGL Carbon, Meitingen, Germany
- University of Victoria, Victoria, BC, Canada

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Fiscal Year (FY) 2011 Objectives

- Develop advanced physical models for water transport and generation, and conduct material and cell characterization experiments.
- Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a proton exchange membrane (PEM) fuel cell.
- Encapsulate the developed models in a modeling and analysis tool for cell design and future application.
- Demonstrate improvements in water management in cells and short stacks.

Technical Barriers

This project addresses the following technical barriers from the Fuel Cells section of the Fuel Cell Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) Durability
(D) Water Transport within Stack
(E) System Thermal and Water Management
(G) Start-up and Shut-down Time and Energy/Transient Operation

Technical Targets

This project addresses fundamental issues in water transport within the fuel cell stack. The resulting understanding will be applied toward the design of stack components and operating strategies that enable meeting the 2015 targets for transportation fuel cell stacks operating on direct hydrogen:

- Stack power density: 2,000 W/L
- Cold start-up time to 50% rated power @ 20°C: 5 secs
- Unassisted start from low temperature: -40°C

FY 2011 Accomplishments

- Predicted design and operating condition sensitivity observed in experimental measurements of wet pressure drop for two-phase flows in channels and gas diffusion layers (GDLs). Applied models to screen channel and cell design for effective water management.
- Integrated membrane water transport models with the computational fluid dynamics (CFD) two-phase cell scale models. Demonstrated improved agreement with measured current density profiles and qualitative agreement with trends in measured liquid water distribution.
- Developed a technique for reproducible, controllable hydrophobic treatment of GDL media that results in less water retention and fewer transport limitations than the treatments applied to commercially available materials.

Introduction

Water management in PEM fuel cells is challenging because of the inherent conflicts between: supplying adequate water to establish and maintain the membrane electrical conductivity, removing the water produced by the electrochemical reactions at the cathode, and uniformly distributing the gaseous reactants at catalyst surfaces near the membrane to effectively utilize these

costly catalysts. As power density of the cells increases, more water will be generated within the same cell volume. Therefore, increasing power density requirements will drive a greater need for design tools incorporating an improved understanding of how liquid water is transported within fuel cells. An additional barrier to widespread use of fuel cells for automotive power is the performance degradation caused when liquid water freezes within the cells. Optimizing water management to influence where the liquid water remains at shutdown is a promising path to improving cold starting capabilities and freeze-thaw reliability.

This project is intended to improve fundamental understanding of water transport within a PEM fuel cell, and capture that knowledge in design tools capable of assisting the industry to meet targets for increased power densities and improved cold-start performance. To achieve these objectives, the project is focused on developing predictive models for water transport in GDL materials, characterizing materials for model inputs and verification, implementing the resulting understanding in engineering design tools, and validating the resulting design tools against fuel cell performance data and in situ diagnostics of water distribution within operating fuel cells.

Approach

To meet the high level objectives of improving the fundamental understanding of water transport in PEMFCs and demonstrating improved performance, the team will integrate experimental characterization with model development and application. The initial focus of the experimental characterization was on measuring relevant physical and transport properties of the GDL materials typically placed between the catalyst and reactant flow channels. Diagnostic and characterization studies have transitioned to water and two-phase (water and air) fluid transport properties of GDL materials and analysis of water transport across material interfaces and in fuel cell channels. The related modeling studies follow a similar progression, with initial emphasis on microscale simulations of single fluid and two-phase transport within GDL materials. The simulations allow us to analyze key effects such as the impact of the microstructure and surface treatment of the solids within porous GDL materials on the two-phase water and gas transport. The knowledge gained from the materials characterization and microscale simulations is being used to develop models suitable for incorporation into an engineering design tool for fuel cell scale analysis of reactant and water transport coupled with power generation. The verification of these models and the resulting design tool will be accomplished by comparing predicted and measured effects of material and operating conditions on cell performance and water distribution within the cell. Applying our models to screen and improve water management strategies, then testing the resulting concepts in prototype fuel cells, will further demonstrate our improved fundamental understanding and validate the resulting design tools.

Results

In this fourth year of research, the emphasis has been on validation of the developed simulation tools and models for fuel cell performance and water transport during operation, application of the modeling tools to evaluate water management and related effects for varying designs and operating conditions, and further development and testing of approaches to improve water management.

The model solution approaches for two-phase flow of liquid water and gases were improved to better address flow across the interfaces between the porous GDLs and the gas channels. CFDRC then simulated two-phase pressure drop experimental studies performed at Ballard, in order to evaluate the current status of the models. This study was intended to gauge the impact of improvements in both the fluid dynamics algorithms, and better understanding of appropriate model setup and property values. The model setup was improved by slightly refining the computational grid, improving the grid node distribution for more uniform computational cell aspect ratios and smoother transitions from fine to coarse regions. Model implementation and solution algorithm improvements for the energy equation could also affect these results, since the Ideal Gas Law was used for gas phase density and the energy equation solution and convergence affect the gas phase density and fluid dynamics. The model was tested against measured pressure drops in the Generation 2 experimental fixture at Ballard, which is more repeatable than the original apparatus due to better sealing. In these experiments, water was injected into a GDL at a constant flow rate mimicking liquid water formation and transport into the channels during cell operation. The air flow rate through the channel was fixed, and pressure drops were measured as a function of time and flow rates. The models predicted the trends in wet pressure drop with operating conditions, Figure 1a, which we were able to capture with earlier models. These models also demonstrated the correct trend for the wet pressure drop response to design variations, particularly changing the channel aspect ratio, Figure 1b, unlike the earlier models.

Ballard has continued to evaluate and apply the simulation tools for a number of cell designs. The numerical stability and accuracy improvements over the last year have enabled an increasing use of computational studies of liquid water effects in non-operational single cells and stacks. The single-channel studies at Ballard demonstrated that the models can accumulate sufficient water in channels to reproduce experimentally observed wet pressure drops. Ballard has also applied the models to two-phase flow in fuel cell stacks, investigating manifold design and flow mal-distribution among as many as 28 parallel channels. The qualitative trends observed in the stack studies are also consistent with experimental observation, particularly the excess air flow required to prevent liquid water from affecting performance. In both the models and experimental stack characterization, it is air stoichiometry and performance in ‘end’ channels that typically suffer

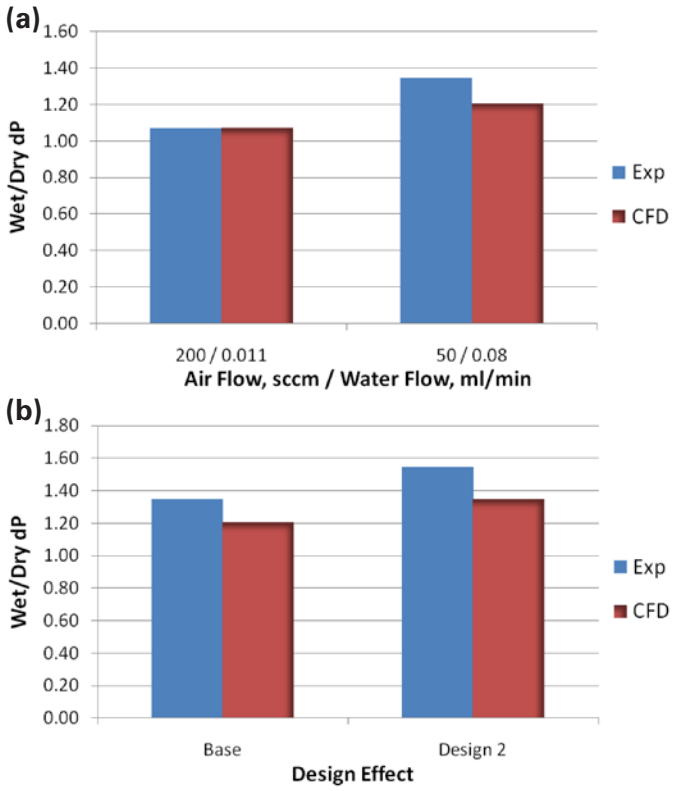

FIGURE 1. Comparison of Predicted and Measured Two-Phase Pressure Drops in Base Channel Design (a) as a Function of Operating Conditions, and (b) at Low Stoichiometry (50/0.08 Flows) Conditions as Function of Channel Design

the greatest reduction in air flow when liquid water in the channels affects performance.

The improvement and evaluation of the two-phase models integrated with electrochemistry, heat transfer, phase change, and water sorption and transport within the membrane has continued. One key model improvement over the past year is improved coupling with the widely used Springer model for transport of water within the membrane [1]. The example experimental data and simulation results presented here are for a three-dimensional model of an operational Ballard MK902 cell, with the simulations including the Springer model. Although this cell has been used previously for model evaluation because of the detailed diagnostic data and past modeling results available for comparison, in this case the experiments were performed at Ballard during the past year. The base operating conditions were cathode stoichiometry 1.8, anode stoichiometry 1.6; relative humidities of the inlet streams cathode 87%, anode 46%; cathode oxidant inlet temperature 65°C, fuel inlet temperature 75°C; and pressure 3 atmospheres in both channels. Model input properties were primarily from historical analysis and fitting at Ballard and CFDRC, with GDL properties updated based on our earlier characterization and a modified capillary pressure function extracted from the measurements of Sole [2]. A residual

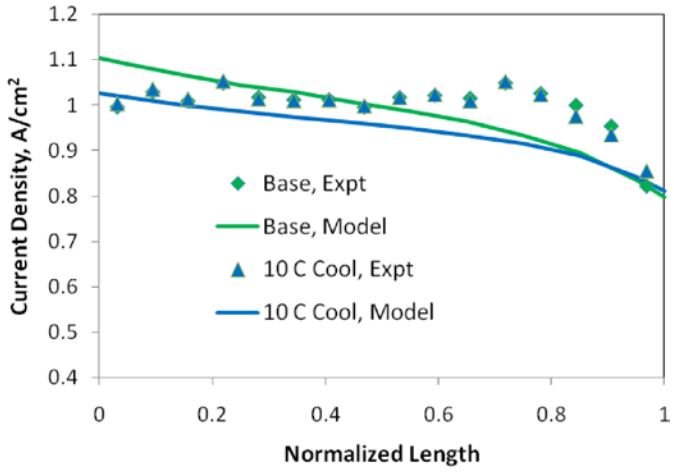

FIGURE 2. Comparison of Predicted and Measured Current Density Profiles for Base and 10°C Cooler Operating Conditions at 1 A/cm^2

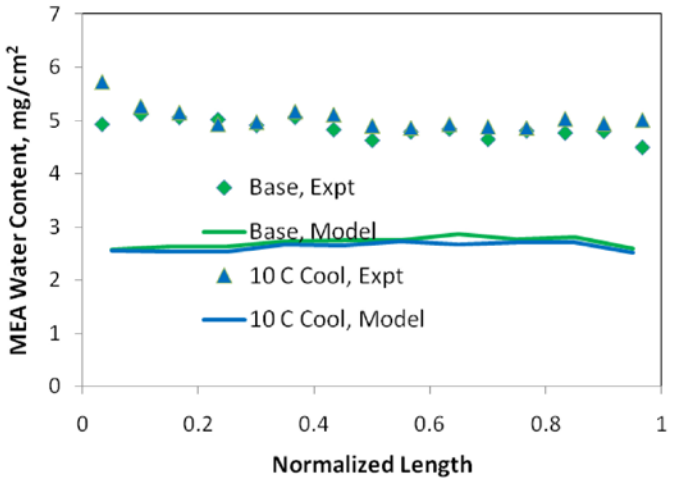

FIGURE 3. Comparison of Predicted and Measured MEA Water Content Profiles for Base and 10°C Cooler Operating Conditions at 1 A/cm^2

saturation of 0.2 was used to obtain the normalized liquid water saturation. Comparison of the predicted and measured current density profiles for the base operating conditions and for 10°C cooler operation, expected to result in additional liquid water, is shown in Figure 2. The experimental data has a large constant current density region along the length of the cell, as opposed to the model results which indicate decreasing current density in the direction of cathode gas flow. The membrane electrode assembly (MEA) water content profiles are more uniform with position in the cell, as shown in Figure 3. Although the prediction is approximately half the measured water mass, the model is capturing the trend of a relatively uniform distribution and little variation of water content between the two operating conditions.

Techverse developed an electrophoresis-based approach for impregnating GDL materials with Teflon®. Various forms

of this treatment are widely used to make the materials hydrophobic, i.e. non-wetting. The samples prepared with the electrophoresis technique consistently have a higher breakthrough pressure than commercially available papers with equivalent Teflon® loading. The materials treated by the developed electrophoresis approach also consistently have a lower residual saturation, indicating a smaller amount of water trapped inside the media. The air permeability of partially saturated samples tends to show greater permeability and less water saturation for a given air flow rate in the Techverse samples. All of these characterization results are consistent with the microscopic imaging analysis, Figure 4, which shows a more uniform Teflon® distribution over the fibers of the GDL in the Techverse samples generated by electrophoresis than in the samples generated by typical commercial production techniques. BCS Fuel Cells prepared fuel cells from the Techverse treated GDLs and measured cell performance. Although the initial tests demonstrated slightly higher electrical contact resistance between the GDL and landings than the control materials, performance improved relative to the control samples as current density was increased. A method for adding a micro-porous layer to the GDLs must be developed to more thoroughly evaluate the Techverse materials, and that process is currently under development.

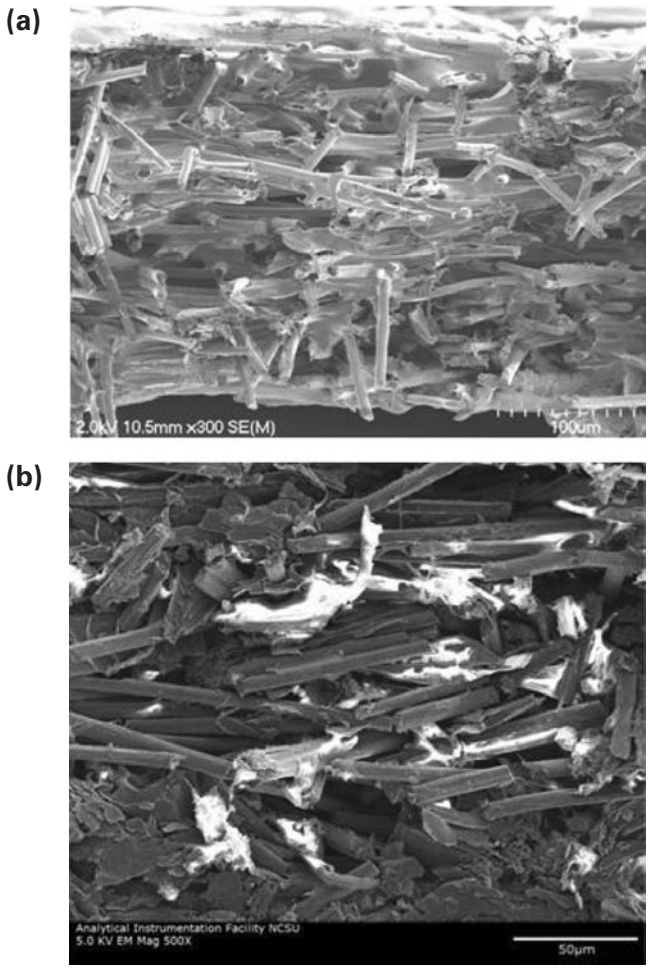

FIGURE 4. Micrographs of (a) Electrophoresis Process Teflonated GDL Material, and (b) Commercially Available Teflonated GDL Material

Conclusions and Future Directions

During the past year, we have demonstrated prediction of liquid water effects for two-phase flows in fuel cell microchannels and begun application to water management issues in cell and stack level component design. A promising materials modification has been developed, increasing the hydrophobicity of GDL materials to reduce water retention and related decreases in cell performance. Specific accomplishments for the past year include:

- Predicted design and operating condition sensitivity observed in experimental measurements of wet pressure drop for two-phase flows in channels and GDLs, applied models to screen channel and cell design for effective water management.
- Integrated membrane water transport models with the CFD two-phase cell scale models, demonstrated improved agreement with measured current density profiles and qualitative agreement with trends in measured liquid water distribution.
- Developed a technique for reproducible, controllable hydrophobic treatment of GDL media that results in less water retention and fewer transport limitations than the treatments applied to commercially available materials.

The key activities planned for the balance of the project are to complete validation of the water transport models based on data gathered during optimization studies, and to make recommendations for water management improvement including operating strategies and GDL materials modifications.

FY 2011 Publications/Presentations

1. S. Mukherjee, A. Gidwani, A. Roy, J. Vernon Cole, K. Jain, C. Bapat, and R. Thoms, "Multiphysics Simulation of Hydrogen PEM Fuel Cell," ECS Trans. 28 (27), pp. 93 – 102 (2010).

2. J. Vernon Cole, "Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization," Proceedings of the DOE Hydrogen and Fuel Cells Program Annual Merit Review, Crystal City, Virginia, 2011, http://www.hydrogen.energy.gov/pdfs/review11/fc030_cole_2011_o.pdf.

References

1. T.E. Springer, T.A. Zawodzinski, and S. Gottesfeld, *Journal Of The Electrochemical Society* **138**, 2334-2342 (1991).

2. Joshua D. Sole and Michael W Ellis, in *ASME 2008 6th International Conference On Fuel Cell Science, Engineering and Technology*, pp. 829-840, ASME, Denver, CO (2008).