V.F.5 Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization

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Subcontractors:
- 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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Project End Date: May 31, 2012

Fiscal Year (FY) 2012 Objectives

- Complete cell-scale model testing and validation against steady state and transient operational cell data.
- Complete fuel cell water transport model improvements and code package development to include two phase flow.
- Complete validation of water transport model based on data gathered during optimization studies, and make recommendations for water management improvement including operating strategies and gas diffusion layer (GDL) materials modification.

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:

(C) Performance

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 2017 targets for transportation fuel cell stacks operating on direct hydrogen:

- Stack power density: 2,250 W/L
- Cold start-up time to 50% rated power @ 20°C: 5 secs
- Unassisted start from low temperature: -30°C

FY 2012 Accomplishments

Specific accomplishments for the past year include:

- Validation of key two-phase (liquid and vapor) flow effects against relevant benchmarks such as channel flow over a porous slab, impinging flow on porous media, and transient flows resulting from local injection of the secondary phase.
- Demonstration of improved agreement with measured polarization curves in the mass transfer limited regime, and significant improvement in the qualitative nature of the predicted liquid water distribution due to several numerical algorithm improvements.
- Completion of the software package development, including: transfer and integration of the model solver software code; addition of model options and parameter inputs to the graphical user interface for model setup; and outputs for post-processing results.

Introduction

Water management in polymer electrolyte membrane (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 fundamental understanding of water transport in PEM fuel cells 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 final 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, and on inserting the developed capabilities into the commercially available version of the multiphysics software utilized in this work.

The model solution approaches for two-phase flow of liquid water and gases were further improved to better address flow across the interfaces between the porous GDLs and the gas channels. The treatment of those interfaces was modified to enforce the pressure and stress matching condition suggested by Beavers and Joseph [1], and by Betchen et al. [2]. In this form, a part of the normal stresses is absorbed by the porous solid, not the fluid in the porous media. A benchmark case relevant to fuel cell operation, the Beavers-Joseph problem with flow in a channel that is segregated into an open and porous region, was used to validate the implementation. As seen in Figure 1, the improved boundary condition treatment results in excellent agreement for the velocity profile as a function of vertical position in the channel and porous layer, without spurious velocity oscillations. The two-phase results are equivalent to the single-phase results after scaling the superficial velocity for the phase fractions. This improvement removed velocity oscillations at the interface which were introducing numerical noise and slowing overall convergence of the models.

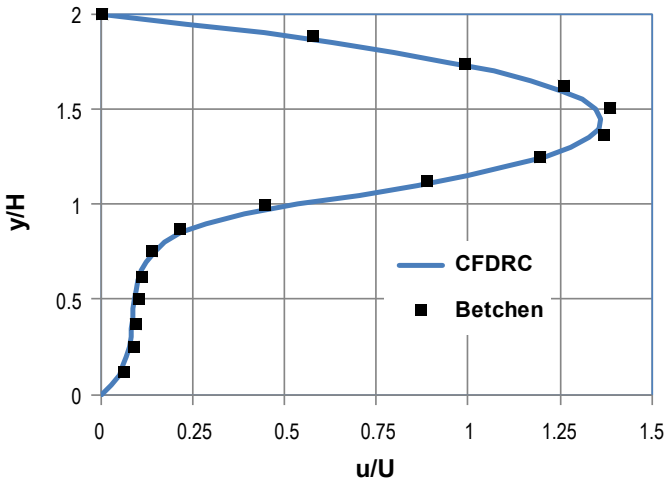

FIGURE 1. Comparison of velocity profile as a function of vertical position between benchmark simulations (symbols) [2] and CFD Research Corporation results (curve) for Beavers-Joseph problem. Porous region is below y/H=1, open channel above.

Model testing against operational fuel cell data has continued to show quantitative and qualitative improvement in the predictions. Ballard experiments for characterization of the membrane electrode assembly (MEA) used in current and next-generation cells have been utilized for some of these model evaluations. The experiments are performed in a small test cell designed to have minimal resistance losses outside the MEA, and operated under high stoichiometry conditions to reduce the effects of reactant depletion on the measured performance. An example measured polarization curve is shown in Figure 2, along with simulation results for the full two-phase model and a simpler single-phase model with no liquid water formation. The cell performance was obtained during 60°C operation with a 100% relative humidity cathode feed, and model parameters for the catalyst kinetics were extracted from a reduced model that only considers the cathode GDL and catalyst layers in detail [3]. The developed two-phase flow models for liquid water transport reduce the cell performance at higher current densities, and bring the predicted polarization curve closer to the experimental values.

The predicted liquid water distribution in the cathode GDL for an 85% relative humidity cathode feed, Figure 3, has a similar range to earlier predictions but is qualitatively improved with much less numerical noise. The liquid water is preferentially formed under the landings, and in the downstream portion of the cathode, due to the temperature and water vapor distributions. Model improvements causing the reduction in numerical noise relative to earlier results include the reformulation of the channel-GDL interface condition described above, a more detailed numerical treatment of the liquid water fraction effect on the phase change rate, and extending the capillary pressure functions to capture both hydrophobic and hydrophilic regimes for materials with a non-zero residual water saturation.

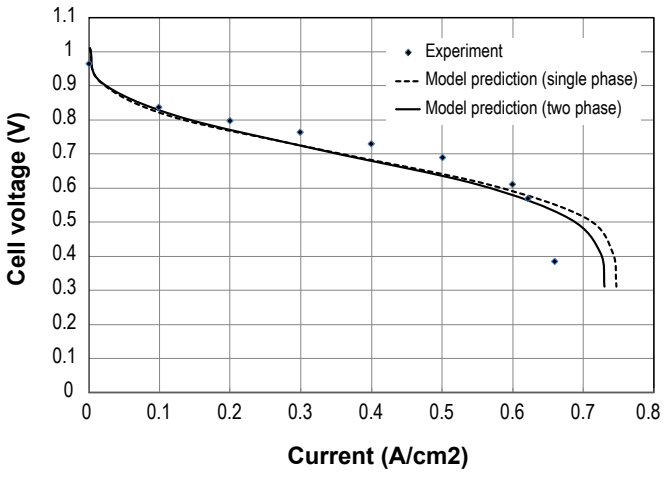

FIGURE 2. Comparison of experimental polarization curve, detailed model with single-phase flow, and detailed two-phase model prediction at 60°C, 100% relative humidity operation.

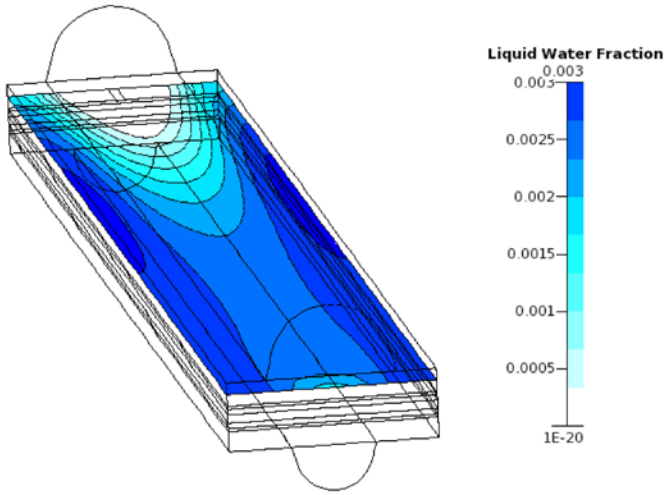

FIGURE 3. Predicted liquid water distribution in cathode GDL mid-plane for 70°C, 85% relative humidity, 1 A/cm^2 operation.

The capabilities for predicting liquid water transport effects developed in this work have been inserted into the commercially available version of the computational fluid dynamics-ACE+ multiphysics software that has served as the development framework. In addition to incorporating the model capabilities, ESI Group and CFD Research Corporation have designed and implemented the appropriate changes to the user interface and property databases. The graphical user interface used to define the models now includes inputs for key properties such as capillary pressure models, relative permeability functions, and models for calculating evaporation/condensation phase change. Printed and graphical results have also been extended to allow detailed analysis of the results.

Conclusions and Future Directions

During the past year, we have further improved and validated the developed models for predicting liquid water and two-phase flow effects in fuel cells. Fundamental capabilities of the models have been validated, and numerical algorithm changes have resulted in improved robustness and convergence. Specific accomplishments for the past year include:

- Validation of key two-phase (liquid and vapor) flow effects against relevant benchmarks such as channel flow over a porous slab, impinging flow on porous media, and transient flows resulting from local injection of the secondary phase.
- Demonstration of improved agreement with measured polarization curves in the mass transfer limited regime, and significant improvement in the qualitative nature of the predicted liquid water distribution due to several numerical algorithm improvements.

- Completion of the software package development, including: transfer and integration of the model solver software code; addition of model options and parameter inputs to the graphical user interface for model setup; and outputs for post-processing results.

The most significant open issue remaining from this project is thorough evaluation of the GDL treatment approach developed by our partner Techverse during the latter stages of this project.

FY 2012 Publications/Presentations

1. 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, 2012, http://www.hydrogen.energy.gov/pdfs/review12/fc030_cole_2012_p.pdf.

References

1. G.S. Beavers, D.D. Joseph, Boundary conditions at a naturally permeable wall, *Journal of Fluid Mechanics* **30**, 197-207 (2006).

2. L. Betchen, A. Straatman, B. Thompson, A Nonequilibrium Finite-Volume Model for Conjugate Fluid/Porous/Solid Domains, *Numerical Heat Transfer: Part A: Applications* **49**, 543-565 (2006).

3. Andrew J. Desouza, Radu Bradean, Virginia Branzea, Stephen Hamada, Joerg Kleemann, Herwig Haas, Joy Roberts, and Emerson Gallagher, in *214th ECS Meeting, Volume 16, Issue 2, Proton Exchange Membrane Fuel Cells 8*, edited by Thomas F. Fuller, K. Shinohara, V. Ramani, P. Shirvanian, H. Uchida, S. Cleghorn, M. Inaba, S. Mitsushima, P. Strasser, H. Nakagawa, H. Gasteiger, T. Zawodzinski, and C. Lamy (ECS, Honolulu, HI, 2008), pp. 35-44.