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

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

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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 Hydrogen, Fuel Cells and Infrastructure 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 is addressing 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 2010/2015 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

Accomplishments

- Characterized key physical and transport properties for gas diffusion layer (GDL) materials, specifically effective capillary pressure as a function of water saturation and air permeability of partially saturated materials.
- Demonstrated the possibility of identifying the onset of flooding in a self-humidified cell by monitoring internal resistance via the current interruption technique, and began characterizing the sensitivity of both self-humidified and industry-standard cells to materials and operating conditions.
- Developed and validated Lattice Boltzmann Method (LBM) tools for predictive simulation of single-phase and two-phase flow with porous media; applied the LBM to analyze GDL microstructure impact on transport properties and to improve understanding of material characteristics controlling water transport within and through GDL 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 the fundamental understanding of water transport within a PEM fuel cell, and capture that knowledge in design tools capable of assisting the industry 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

The project will initially focus on characterizing transport properties of representative materials, particularly the GDL materials typically placed between the catalyst and reactant flow channels, and developing models for two-phase transport within bulk materials and across material interfaces. The initial efforts are planned to generate data characterizing the water transport properties of representative GDL materials. This is being accomplished through experimental measurements of average properties of materials, particularly capillary pressure and relative permeabilities during two-phase flow. In conjunction with this data, we are developing and applying predictive LBM models 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 will be 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 first year of the research, the emphasis has been on experimental characterization of representative GDL materials and development of models of transport within these materials. Extension of the established computational fluid dynamics (CFD)-based fuel cell engineering design tools to enable compatibility with the developed physical models was initiated, but the modeling effort was mainly directed toward predictive models resolving the microstructure of porous GDL media.

RTI has measured key material properties governing two-phase transport for baseline GDL materials provided by SGL Carbon, specifically SGL 24, 25, 34, and 35 BC materials. Capillary pressure has been estimated by performing imbibing and draining experiments with known volumes of water displacing the air in initially dry samples. As illustrated by the sample data of Figure 1, this approach provides both an estimate of the capillary pressure, and the maximum fraction of the pore volume filled by water before connected pathways for transport allow water to break through the materials. We have also begun to characterize the permeability of these GDL materials when partially saturated. In these experiments, air pressure is applied to wet sample until breakthrough occurs, then the pressure drop is measured at varying air flow rates to enable calculation of the gas phase permeability of the partially saturated media.

The modeling efforts at CFDRC and ESI have emphasized development and application of a LBM

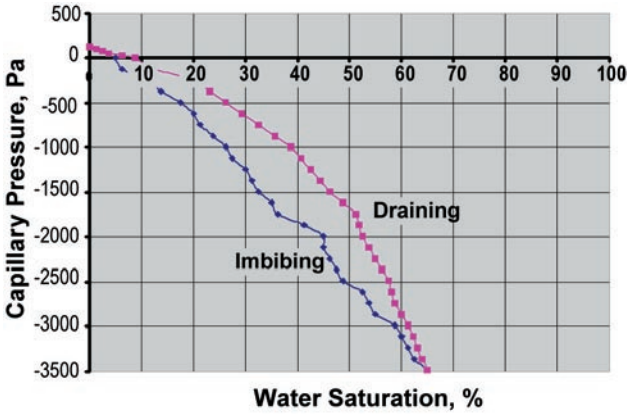

FIGURE 1. Capillary Pressure as a Function of Water Saturation for SGL 35 BC GDL Material

simulation capability for prediction of two-phase transport in porous media and microchannels. An LBM code capable of addressing single-phase flow in porous media was developed, and the model implementation was validated against benchmark tests with known solutions such as flow in a channel and flow through a packed bed of spherical particles. The predictions were also shown to compare favorably to published single-phase LBM predictions of gas permeability in fuel cell GDL materials [1]. Before extending the model to two-phase transport, the validated model was applied to assess the feasibility of controlling the transport properties of GDL materials through preferential orientation of the solid fibers. The results, Figure 2, indicate that by modifying the orientation of the GDL fibers it is possible to control the in-plane permeability without significantly modifying the through-plane permeability. The LBM model was then extended to address two-phase transport of liquids and gases, and the two-phase model was validated against relevant benchmark tests. The two-phase model was then applied to analyze water imbibing into, and consequently breaking through, microstructures representative of GDL materials. The initial results, Figure 3, demonstrated qualitative agreement with the commonly observed trend for preferential breakthrough locations [2-4]. Subsequent efforts in this area of predictive microscale modeling have been directed toward generation of representative microstructures of representative materials. We are evaluating both laser-scanning microscopy, which provides limited depth resolution, and X-ray tomography, in order to gather the information necessary for constructing porous microstructures representative of the characterized GDL materials.

Development of the fuel cell scale engineering design and analysis models was initiated, although the principle effort in this area will come in the next year of the project. The models will utilize the infrastructure developed during previous research, primarily a multiphysics CFD software package using the finite volume discretization technique. The principle effort in this year has been to improve the fundamental two-phase flow modeling algorithms, in order to achieve the stability and robustness necessary for practical application later in the project. Significant improvements in convergence and stability during simulation of two-phase flows in microchannels have been obtained by reformulating the equations for conservation of mass in each phase.

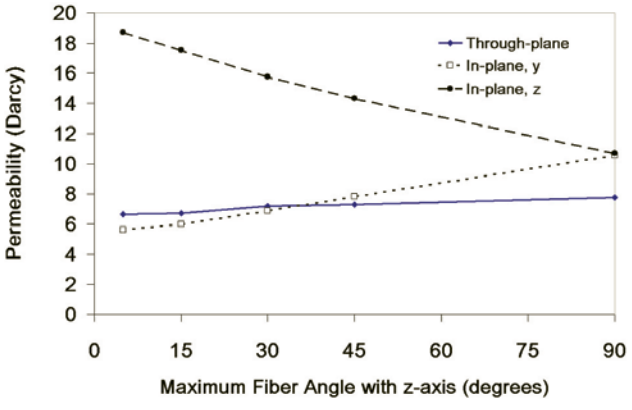

FIGURE 2. LBM Predicted Directional Permeability Variation with Fiber Orientation in a Fibrous GDL Material

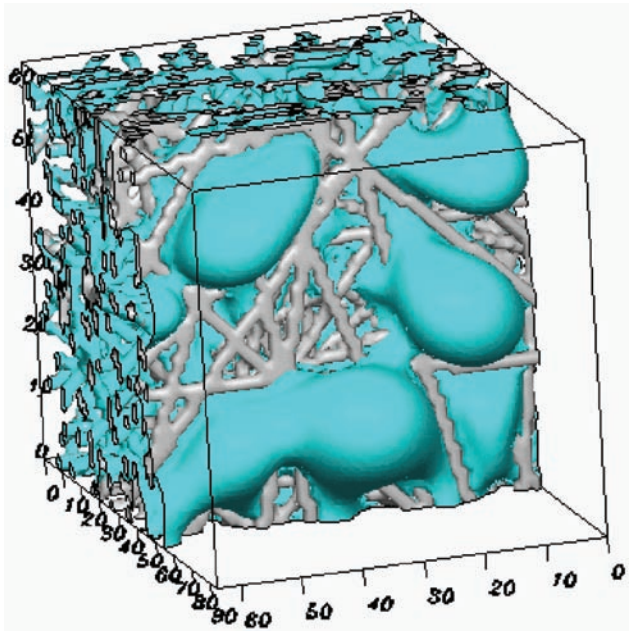

FIGURE 3. Liquid Water Surface Emerging from Preferential Locations on the Surface of a Fibrous GDL Material

Characterization of water transport within operational fuel cells has been initiated using two distinct cell architectures. BCS used small-scale fuel cells, 25 cm^2 active area, with a unique self-humidified membrane electrode assembly (MEA) to assess the impact of a variety of GDL materials on performance. The use of current interruption techniques to monitor the internal resistance of these self-humidified cells has been evaluated, and this appears to be a promising approach for monitoring the average water content within the MEA and possibly for identifying the onset of flooding. For fuel cell designs more representative of the industry standard, Ballard has assembled a comprehensive package of in situ diagnostic data measured during recent internal research programs. This data includes the effect of operating conditions and materials on a variety of key quantities such as spatial distribution of water inside the MEA, volume fraction of liquid water in gas channels as a function of position, and spatial variations of current density.

Conclusions and Future Directions

In the past year, we have established characterization techniques and predictive modeling capabilities that are advancing the understanding of water transport within fuel cells. Specific accomplishments include:

- Characterizing key physical and transport properties for representative GDL materials.
- Demonstrating self-humidified cell diagnosis by infrared, gathering performance data and diagnostics for effects of materials and operating conditions on water distribution within operating cells.
- Developing and validating LBM models for single-phase and two-phase flow with porous media; then applying those models to analyze microstructure impact on permeability and liquid water breakthrough.

In particular, the LBM approach has been demonstrated to be a valuable tool for analyzing transport within the complex GDL structures. This method provides a valuable complement to experimental characterization techniques, and appears capable of providing detailed information to both assess materials based approaches to improved water management and support development of engineering models.

Key activities planned for the coming year include:

- Perform diagnostic experiments and apply the LBM models to improve understanding of water transport across the GDL-gas channel interface.
- Develop the necessary models for GDL material transport properties, and two-phase transport across the GDL-channel interface, and implement them into the cell-scale models.
- Assess the performance of the developed models by comparison with diagnostic data from PEM fuel cells.

Future work will consist primarily of testing the models against diagnostic data and improving them as necessary, then demonstrating an improved understanding of the key factors controlling water transport by developing improved water management approaches.

References

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