V.F.3 Development and Validation of a Two-Phase, Three-Dimensional Model for PEM Fuel Cells

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Project End Date: October, 2012

Fiscal Year (FY) 2012 Objectives

- Perform the validation of the three-dimensional (3-D), partially two-phase, single-cell polymer electrolyte membrane (PEM) fuel cell model.
- Validate model under real-world conditions and architectures using data from Ballard and Nissan for non-automotive and automotive applications.
- Validate fully two-phase, 3-D cell model with micro-porous layer effect using neutron imaging data.
- Generate test suite for PEM fuel cell model and create user manual.

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:

(B) Cost

(C) Performance

Technical Targets

Since the validated PEM fuel cell model developed in this project can be employed to improve and optimize the design and operation of PEM fuel cells, insights gained from applying the model will help meet the following technical targets:

- Cost: $15/kW for transportation fuel cell stacks.
- Performance: 2,250 W/L or 65% energy efficiency for transportation fuel cell stacks.

FY 2012 Accomplishments

- Model validation using polarization and current distribution data obtained by LANL using a 10x10 segmented cell was performed. At 80ºC model current distribution prediction error was <15% root mean square (RMS) error and +/-30% local error. At 60ºC errors were <20% RMS and between -40/+60% local error.
- Nissan collaboration resulted in new sub-models for low Pt loading. A model for micro-resistance was applied for performance prediction of low-Pt loaded catalyst layers, with excellent performance agreement up to 2.2 A/cm^2.
- Single-channel models for Ballard stack and single-cell architecture have been built. Models are being used for validation of down-the-channel current, temperature and liquid water distribution.
- Demonstration of the two-phase model for predicting liquid water in a form comparable to neutron imaging studies of liquid water for in situ fuel cells. Qualitative validation against experimental through-plane liquid water profiles.
- Channel liquid water predictions were demonstrated using the fully two-phase model on the LANL 10x10 segmented cell flow field.
- Water saturation convergence at both anode and cathode sides is greatly improved for the latest code with simulation time to convergence reduced by 60%.
- A user manual has been documented for the two-phase code developed and demonstrated in this project.

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Introduction

As PEM fuel cell (FC) technology matures and enters the stage of commercialization such that the industry strives to achieve desired performance and durability and reduce costs, process design and optimization become increasingly important and indeed critical. Modeling and simulation can provide guidance in PEMFC design and optimization and thus help accelerate the commercialization of PEMFC technology. Despite tremendous research efforts and a large number of models published in the literature (see Chen and others [1] and references therein), a comprehensive, multi-physics computer model suitable for practical use by PEMFC engineers and designers, particularly in transportation and stationary applications, is still lacking.

The objectives of this project are twofold: 1) to develop and validate a two-phase, three-dimensional transport model for simulating PEMFC performance under a wide range of operating conditions; and 2) to apply the validated PEMFC model to identify performance-limiting phenomena or processes and develop recommendations for improvements so as to accelerate the commercialization of fuel cell technology. To achieve these two objectives, a multi-institutional and interdisciplinary team with significant experience in modeling PEMFCs and in measuring model-input parameters and model-validation data has been assembled. This team is led by SNL, and it includes another national laboratory (LANL), a university (PSU), and two PEMFC manufacturers (Nissan and Ballard). In addition to developing and validating a two-phase, 3-D PEMFC model, we are also coupling the PEMFC model with Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) [2] (a toolkit for design, optimization, and uncertainty quantification developed by Sandia National Labs) in order to create a computational capability that can be employed for PEMFC design and optimization. This report documents technical progress made in the project during FY 2012.

Approach

Our approach is both computational and experimental. We first develop a two-phase, 3-D, transport model for simulating PEMFC performance under a wide range of operating conditions by integrating the detailed component sub-models; FLUENT (a commercial computational fluid dynamics code) is employed as the basic computational platform. We then validate our PEMFC model in a staged approach using experimental data available from the literature and those generated by team members. Lastly, we plan to apply the validated PEMFC model to identify performance-limiting phenomena or processes and develop recommendations for improvements.

Results

A validation milestone of local current distribution was successfully completed in the first quarter. We compared local current distribution from the model to experimentally measured current distributions (obtained by LANL) from a 10x10 segmented current collector plate on the cathode of a 50-cm^2 cell with serpentine flow field. Agreement with experimental data for cell voltage was within 15 mV for all cases (80ºC and 50/100 relative humidity, RH). At 80ºC, local current distribution agreed with measurements to within 15% RMS and with min/max local errors of -30/30%. However, at 60ºC, RMS error increased to 20% and min/max local errors were -30/60%, indicating overestimation of local current (see Figure 1). A novel feature of our validation approach was the quantification of experimental and model uncertainty and inclusion of this uncertainty into the validation metrics [publications 1-3,6].

The model for local current distribution was used to assess the effect of the fully two-phase model on channel liquid water (the partially two-phase model reported previously assumes only water vapor in gas channels). While the liquid water did not significantly impact the cell performance (polarization curve), a large difference in liquid water *distribution* was seen, as shown in Figure 2. Here we see that in the partially two-phase model, at the cathode gas diffusion layer (GDL)/channel interface liquid water can only appear under the lands (areas not in contact with channels). In contrast, the fully two-phase model predicts a more even distribution of liquid water over the entire lower portion of the cell, with maximum liquid water saturation under the land areas. In addition, a parametric study indicated that liquid water accumulation in the cathode gas channel would increase with increasing RH and decreasing temperature [publications 6,7,15].

Neutron imaging experiments were performed by LANL at the National Institute of Standards and Technology (NIST) facility in order to measure distribution of liquid water in an operating fuel cell. These were done using a special 2.5-cm^2 area cell with a single serpentine channel. A PEMFC model was built for this geometry and a special postprocessing script was used to convert computed

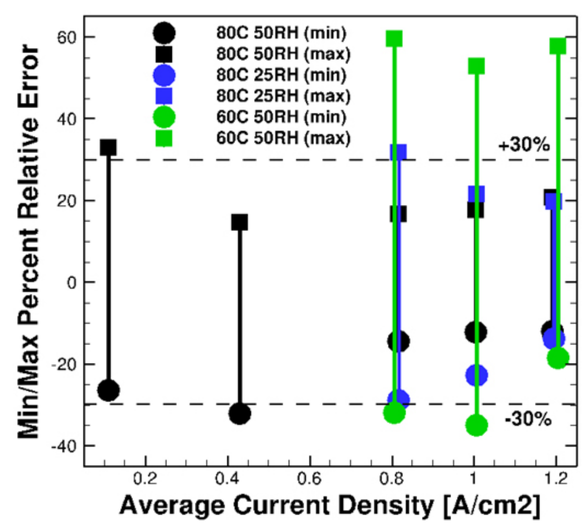

FIGURE 1. Validation of local current distribution (min/max errors) under various temperature, current and RH conditions

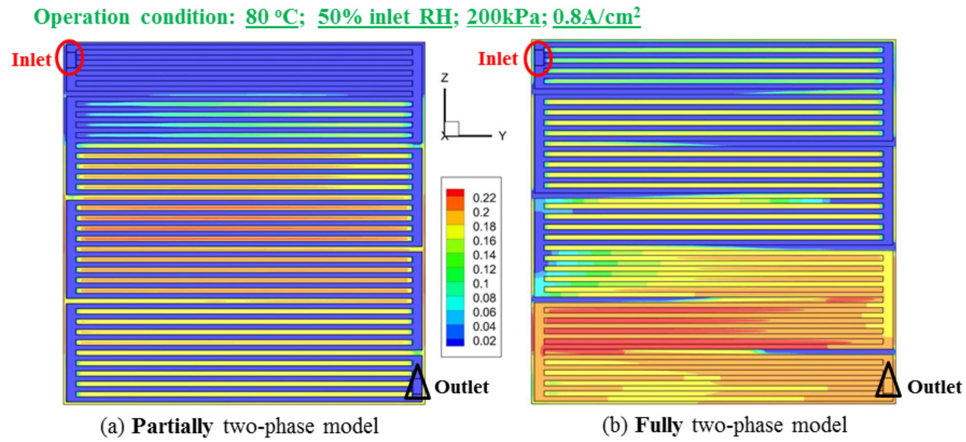

FIGURE 2. Comparison of partially/fully two-phase model using 50-cm^2 flow field used for current distribution validation. Two-dimensional plots of liquid water saturation at the cathode GDL/channel interface.

liquid water in the porous layers (GDL/microporous layer/catalyst layer/membrane) into an equivalent water thickness comparable to the water thickness measured in the neutron beam path. Results from the model compared favorably with the experimental water profiles, at least qualitatively (see Figure 3). However, it is uncertain whether quantitative comparisons of liquid water distribution are currently possible. This question will be pursued in the remainder of this project. [publications 4,5,11]

The code was applied to model two different Ballard fuel cell architectures: 1) a single channel from a full stack and 2) a single channel from a single cell used for parametric studies and neutron imaging of liquid water. The stack model is being used to compare distributions of current and temperature from inlet to outlet. The single-cell model will be used to predict distributions of current, temperature, and liquid water. These models are also being used to identify performance-limiting phenomena or processes.

An engineer from Nissan worked onsite at PSU and helped to develop and implement a new resistance sub-model to improve prediction of cell performance of low Pt loaded catalyst layers. In Figure 4 we show a comparison of model prediction both with and without the new sub-model along with Nissan performance data. The improved predictive

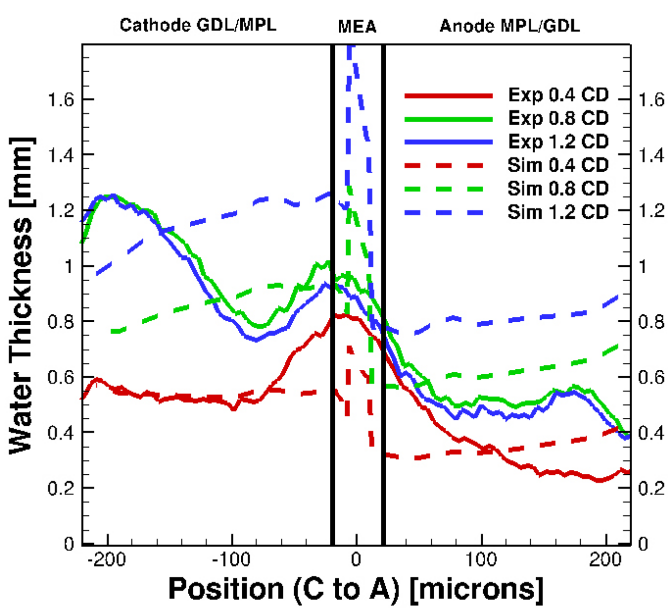

FIGURE 3. Validation of through-plane liquid water distribution model prediction by comparison with LANL/NIST neutron imaging experimental data at 100% RH

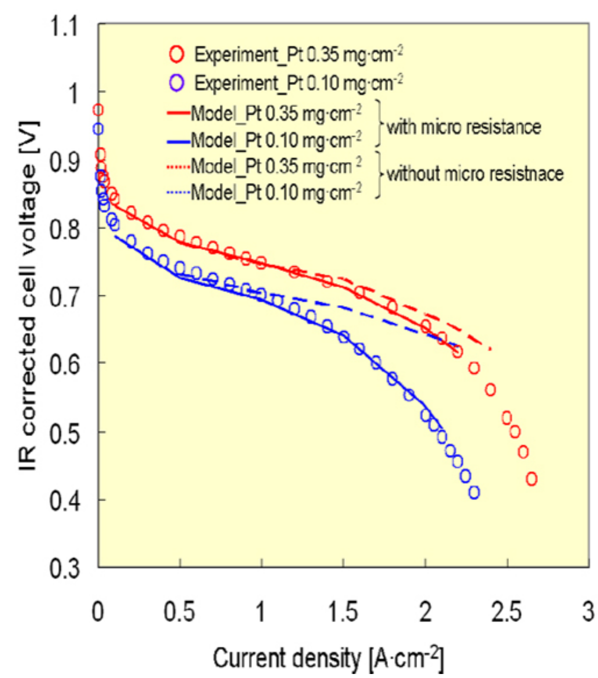

FIGURE 4. Validation of new resistance model for low Pt-loaded catalyst layers using data from Nissan

capability is clear, especially for current density greater than 1 A/cm^2.

The performance of the computer model was improved, so that simulation time is reduced by up to 60%. This was done by improving the implementation of the liquid water transport in the model. In addition, the user manual has been revised and test problems created to facilitate new users of the model. Finally, the scripts used to couple the model with the DAKOTA optimization toolbox [2] were documented and will be supported by Brian Carnes (bcarnes@sandia.gov) at SNL. Requests for information about running the code should be directed to Dr. Chao-Yang Wang (cxw31@psu.edu) at PSU.

Conclusions

- The model can produce current distributions that have quantitative predictive capability, within about 30% local relative error at 80ºC.
- The model's predictive capability for liquid water predictions in porous layers is still only qualitative. Quantitative prediction of liquid water distribution is not yet proven.
- The model is suitable for studies to identify performance-limiting phenomena or processes.

Future Directions

- Complete model validation of liquid water distribution using neutron imaging data.
- Complete validation studies using test data from Nissan and Ballard.

FY 2012 Publications/Presentations

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2. B. Carnes, D. Spernjak, G. Luo, L. Hao, K.S. Chen, C.-Y. Wang, "Validation of a two-phase multidimensional PEMFC computational model using high-resolution current distribution data", submitted to Journal of Power Sources.

3. B. Carnes, "Development and validation of a three-dimensional, two-phase, PEM fuel cell model", presentation at the *2012 DOE Hydrogen Program Annual Merit Review and Peer Evaluation Meeting*, Washington, DC, May 15, 2012, paper #FC027.

4. B. Carnes, K.S. Chen, D. Spernjak, L. Hao, G. Luo, C.-Y. Wang, "Simulation and validation of liquid water transport in fuel cells from neutron imaging experiments", in ASME Proceedings of FuelCell2012, paper #91130.

5. B. Carnes, D. Spernjak, G. Luo, L. Hao, K.S. Chen, C.-Y. Wang, "Validation of a two-phase multidimensional PEMFC computational model using high-resolution neutron imaging data", in preparation.

6. K.S. Chen, B. Carnes, L. Hao, Y. Ji, G. Luo, C.-Y. Wang, Y. Wang, "Toward the development and validation of a comprehensive PEM fuel cell model", in ASME Proceedings of FuelCell2011, paper #54693.

7. K.S. Chen, B. Carnes, L. Hao, G. Luo, C.-Y. Wang, "A three-dimensional two-phase model for simulating PEM fuel cell performance", accepted for publication in the ASME Proceedings of ESFuelCell2012, paper #91302.

8. S.C. Cho, Y. Wang, and K.S. Chen, "Droplet dynamics in a polymer electrolyte fuel cell gas flow channel: deformation and detachment. II: comparisons of analytical solution with numerical and experimental results", Journal of Power Sources (in press).

9. S.C. Cho, Y. Wang, and K.S. Chen, "Droplet dynamics in a polymer electrolyte fuel cell gas flow channel: forces, deformation, and detachment. I: theoretical and numerical analyses", Journal of Power Sources (in press).

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16. Y. Wang, and K.S. Chen, "Modeling of polymer electrolyte membrane fuel cells and stacks", in Fuel Cells Science and Engineering: Materials, Systems, Processes and technologies", First Edition, Edited by Detlef Stolten and Bernd Emonts, Chapter 31, in press (2012).

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2. http://www.cs.sandia.gov/dakota/index.html