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

Ken S. Chen[1] (Primary Contact), Brian Carnes[1], Chao-Yang Wang[2], Adam Weber[3], Rod Borup[4], Atul Kumar[5], Patricia Chong[6]

[1]Sandia National Laboratories
Org. 1516, MS0836, P.O. Box 5800
Albuquerque, NM 8718-0836
Phone: (505) 844-5783
E-mail: kschen@sandia.gov

DOE Technology Development Manager:
Jason Marcinkoski
Phone: (202) 586-7466
E-mail: Jason.Marcinkoski@ee.doe.gov

Subcontractors:
[2] Pennsylvania State University, University Park, PA
[3] Lawrence Berkeley National Laboratory, Berkeley, CA
[4] Los Alamos National Laboratory, Los Alamos, NM
[5] Ford Motor Company, Dearborn, MI
[6] Ballard Power Systems, Burnaby, BC, Canada

Project Start Date: October, 2009
Project End Date: 2013

Objectives

- Develop and validate a two-phase, three-dimensional transport model for simulating proton exchange membrane (PEM) fuel cell performance under a wide range of operating conditions.
- Apply the validated PEM fuel cell model to improve fundamental understanding of key phenomena involved and to identify performance-limiting processes and develop recommendations for improvements.

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

(D) Water transport within the Stack

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:

- Performance: 650 W/L or 50% energy efficiency for automotive applications; 40% electrical energy efficiency for stationary applications.
- Cost: $30/kW for automotive applications and $750/kW for stationary applications.
- Durability: 5,000 hours for automotive and 40,000 hours for stationary applications.

Accomplishments

- Developed a single-phase, three-dimensional (3-D), single-cell model and made significant progress toward meeting the milestone of developing a 3-D, partially two-phase, single-cell PEM fuel cell model.
- Coupled the present PEM fuel cell model with DAKOTA (which is a toolkit for design, optimization, and uncertainty quantification developed by Sandia National Labs).
- Demonstrated the capabilities of the present PEM fuel cell model in case studies.
- Demonstrated utilities of the coupled PEM fuel cell model/DAKOTA capability in case studies.
- Implemented a sub-model for simulating cathode microporous layer (MPL) effect.
- Simulated performance of a PEM fuel cell with zigzag flowfield using the present model.
- Investigated water transport through cathode MPL-gas diffusion layer (GDL) using a pore-network model.
- Developed and demonstrated a sub-model for predicting membrane interfacial resistance.
- Measured pore size distributions of various GDLs with and without MPL.
- Obtained experimental polarization curves for different temperatures, relative humidity (RH), and cell segments.
- Measured axial and radial thermal conductivities of GDLs with various poly-tetrafluoroethylene contents.
- Measured liquid water profiles across GDL-MEA regions using neutron imaging for four different GDLs and two different relative humidities.
- Measured along-channel current and temperature profiles in a 12 kW PEM fuel cell stack.

Introduction

As PEM fuel cell 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 PEM fuel cell design and optimization and thus help accelerate the commercialization of PEM fuel cell technology. Despite tremendous research efforts and a large number of models published in the literature (see Chen et al. [1] and references therein), a comprehensive, multi-physics computer model suitable for practical use by PEM fuel cell engineers and designers, particularly in transportation and stationary applications, remains absent. This mainly is due to the many challenges involved in modeling the PEM fuel cell operation: multiple components and phases, multi-dimensionality, and complex physics with highly coupled transport phenomena and electrochemical reactions. The significantly disparate length scales in transport and the presence of liquid water within the PEM fuel cell when operating under practical current loads, relatively high inlet RH or moderate cell temperature, further add to the modeling challenges.

The objectives of this project are twofold: 1) to develop and validate a two-phase, three-dimensional transport model for simulating PEM fuel cell performance under a wide range of operating conditions; and 2) to apply the validated PEM fuel cell 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 PEM fuel cells and in measuring model-input parameters and model-validation data has been assembled. This team is led by Sandia National Laboratories; and it includes two other national laboratories (Los Alamos National Laboratory and Lawrence Berkeley National Laboratory), a university (The Pennsylvania State University), and two PEM fuel cell manufacturers (Ford Motor Company and Ballard Power Systems). In addition to developing and validating a two-phase, 3-D PEM fuel cell model, we are also coupling the PEM fuel cell model with DAKOTA [2] (which is 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 PEM fuel cell design and optimization. This report documents technical progress made in this project during the first nine months of Fiscal Year (FY) 2010.

Approach

Our approach is both computational and experimental. We first develop a two-phase, 3-D, transport model for simulating PEM fuel cell 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 PEM fuel cell 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 PEM fuel cell model to identify performance-limiting phenomena or processes and develop recommendations for improvements. As mentioned previously, we have assembled a team of leading experts in PEM fuel cell modeling as well as in physical, electrochemical and transport property characterization, and cell diagnostics via segmented cell measurements and neutron imaging – this means that our project team is highly qualified and in an excellent position to carry out the project.

Results

To illustrate the utility of the present PEM fuel cell model, polarization curves for three cell temperatures, RHs at the cathode inlet, cathode back-pressures, and cathode stoichiometric flow ratios, were computed in case studies. Due to space limitation, only the effect of cell temperature on cell voltage is shown here in Figure 1. A schematic of the PEM fuel cell used in these case studies and the geometrical parameters, material properties, and operating conditions are available elsewhere (see Chen et al. [1], Chen [3]). As shown in Figure 1, cell voltage increases with cell temperature. Figures 2a, 2b, and 2c display, respectively, computed 3-D contours of temperature, H_2 concentration in anode flow channel, GDL and catalyst layer, and O_2

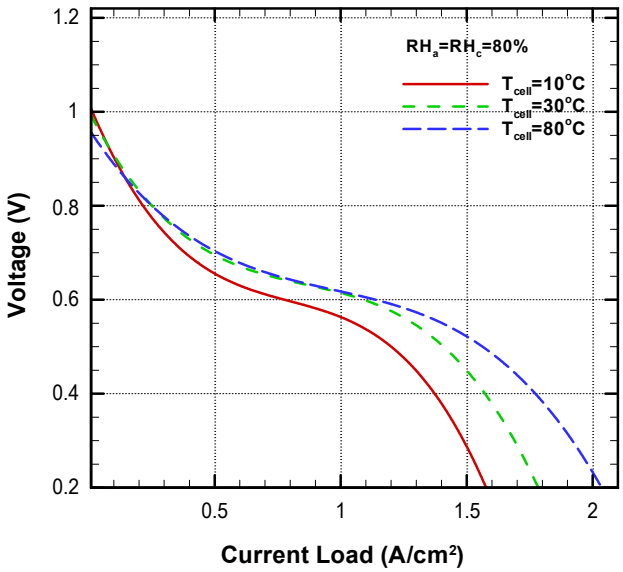

FIGURE 1. Effect of Cell Operating Temperature on Cell Voltage (RH_{anode}=$RH_{cathode}$=80%)

concentration in cathode flow channel, GDL and catalyst layer. It should be noted that H_2 and air flow in a counter-flow fashion: H_2 flows from right to left whereas air from left to right in Figure 2.

To further illustrate its capability, the present PEM fuel cell model was employed to simulate the performance of a PEM fuel cell having a zigzag and trapezoid-cross-sectional flow field. Similar flow field design has already been adopted in practice [4]. Figure 3a shows the computed temperature contours. Figures 3b and 3c display the contours of H_2 and O_2 concentrations at the mid-plane of the anode and cathode catalyst layer, respectively. Though not shown due to space limitation, water content and current density distribution at the mid-plane of the membrane were also computed. In computed results shown in Figure 3, the cell was taken to operate at 200 kPa, 80°C, 1.0A/cm^2, 81% RH, 1.4 anode stoichiometry and 1.8 cathode stoichiometry. The simulated unit cell has an active area of 1.573 cm^2. The gas channels have a trapezoid cross-sectional area of 0.285 mm^2. The zigzag unit length and amplitude are 50 mm and 1.0 mm, respectively.

In addition to developing a baseline PEM fuel cell model, we've also implemented a sub-model of the MPL in order to investigate its effect on cell performance, particularly on water transport. It is known in industrial practices that MPL results in effective water management and improved cell performance. The present MPL sub-model is formulated based on the continuity of capillary pressure and water flux at the catalyst-layer (CL)/MPL and MPL/GDL interfaces. This allows the use of different realistic material parameters for different layers, thus automatically enabling the PEM fuel cell model to handle water transport across different porous layers. Figure 4 shows computed liquid-water saturation profile across the CL-MPL-GDL regions from a case study. Also plotted is liquid saturation for the case when MPL is absent. Clearly from Figure 4, MPL effectively reduces water saturation in the cathode MPL-GDL regions. It should be noted that in the present work, the MPL submodel was implemented in the cathode side only.

Summary and Conclusions

- A single-phase, 3-D, single-cell model for simulating PEM fuel cell performance was developed and the milestone of developing a 3-D, partially two-phase, single-cell PEM fuel cell model is expected to be met by the end of this FY.
- The present PEM fuel cell model was coupled with DAKOTA and this coupled computational

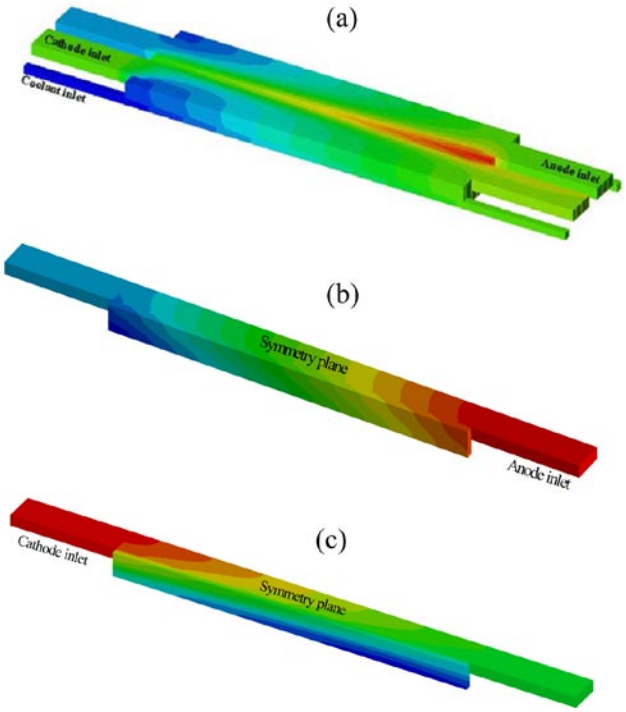

FIGURE 2. Computed 3-D contours: a) temperature; b) H_2 concentration contours in anode channel, GDL and catalyst layer; and c) O_2 concentration contours in cathode channel, GDL and catalyst layer.

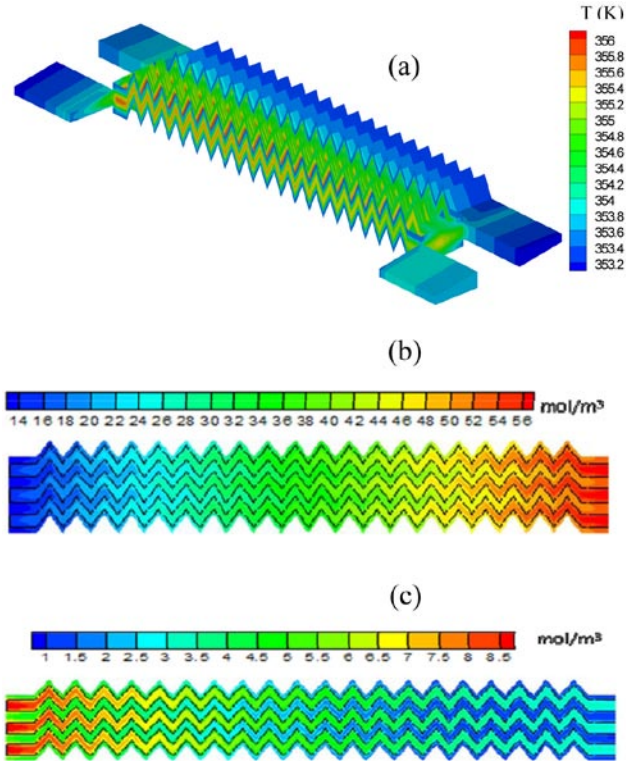

FIGURE 3. Computed contours of a PEM fuel cell with zigzag flowfield: a) temperature; b) H_2 concentration contours in anode catalyst layer; and c) O_2 concentration contours in cathode catalyst layer.

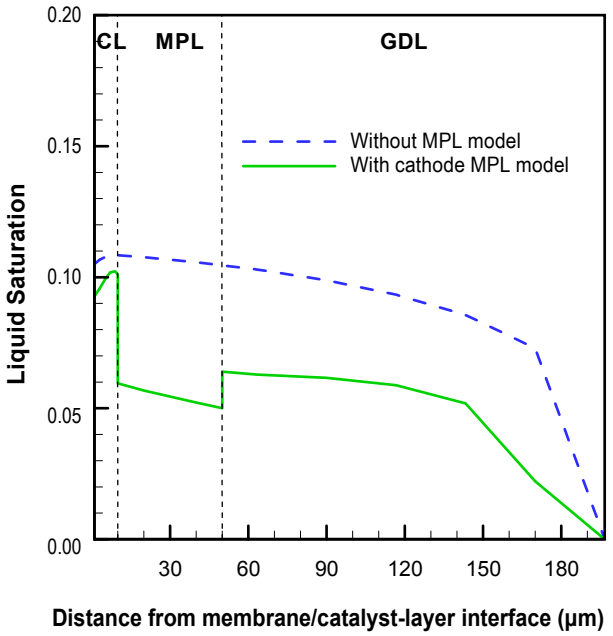

FIGURE 4. Computed Liquid Saturation Profile in the Cathode CL/MPL/GDL Regions

capability will be useful in PEM fuel cell design and optimization.

- A MPL sub-model was implemented for the cathode side and results computed from a case study indicates that MPL effectively reduces water saturation in the cathode MPL-GDL regions.
- The present model was capable of simulating performance of a PEM fuel cell with complex zigzag flowfield having trapezoid cross-section.

Future Directions

- Complete development of a 3-D, partially two-phase, single-cell PEM fuel cell model.
- Complete measurements of model-input parameters and model-validation data in the single-phase operating regime; perform measurements in the partially two-phase operating regime.
- Perform validation of the 3-D, partially two-phase, single-cell PEM fuel cell model.
- Develop a 3-D, fully two-phase, single-cell PEM fuel cell model.
- Develop a sub-model for specifying boundary conditions at the GDL/channel interface.
- Couple PEM fuel cell model with DAKOTA for parameter estimation and uncertainty quantification.

FY 2010 Publications/Presentations

1. K.S. Chen, B. Carnes, F. Jiang, G. Luo, and C.-Y. Wang, "Toward developing a computational capability for PEM fuel cell design and optimization", in ASME Proceedings of FuelCell2010, paper # FuelCell2010-33037.

2. B. Carnes, K.S. Chen, F. Jiang, G. Luo, and C.-Y. Wang, "Systematic parameter estimation and sensitivity analysis using a multidimensional PEMFC model coupled with DAKOTA", in ASME Proceedings of FuelCell2010, paper # FuelCell2010-33038.

3. G. Luo, F. Jiang, C.-Y. Wang, and K.S. Chen, "Numerical Modeling of Micro-porous Layers in a Two-Phase Multidimensional PEM Fuel Cell Model", presented at the 8th Int. Fuel Cell Sci., Eng. & Technology Conf., Brooklyn, NY, June 14–16, 2010; paper # FuelCell2010-33164.

4. F. Jiang, G. Luo, C.-Y. Wang, and K. S. Chen, "Simulation of a PEMFC with Zigzag Flow Field", presented at the ASME FuelCell2010 Conference, paper # FuelCell2010-33108.

5. Y. Ji, G. Luo, and C.-Y. Wang, "Computer Simulation of Liquid Water Transport at Pore Level in MPL and GDL and Their Interface", presented at the FuelCell2010 Conference, paper #33122.

6. B. Kientiz, H. Yamada, N. Nonoyama, and A.Z. Weber, "Interfacial Water-Transport Effects in Proton-Exchange Membranes", *J. Fuel Cell Science & Technology*, in press (2010).

7. G. Luo, Y. Ji, C.Y. Wang and P.K. Sinha, "Modeling Liquid Water Transport in Gas Diffusion Layers by Topologically Equivalent Pore Network", Electrochimica Acta, accepted (2010).

References

1. K.S. Chen et al., "Toward developing a computational capability for PEM fuel cell design and optimization", in ASME Proceedings of FuelCell2010, paper # FuelCell2010-33037.

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

3. K.S. Chen, "Development and validation of a three-dimensional, two-phase, PEM fuel cell model", in 2010 DOE Hydrogen Program Annual Merit Review and Peer Evaluation Meeting Proceedings, US Department of Energy, paper #FC027.

4. S. Kandlikar et al., "Visualization of fuel cell water transport and performance characterization under freesing conditions", in 2008 DOE Hydrogen Program Annual Merit Review and Peer Evaluation Meeting Proceedings, US Department of Energy, paper #FC33.