# V.F.2 Development and Validation of a Two-Phase, Three-Dimensional Model for PEM Fuel Cells

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Project End Date: September 2012

## Objectives

- Develop and validate a two-phase, three-dimensional (3-D) transport model for simulating proton exchange membrane fuel cell (PEMFC) performance under a wide range of operating conditions.
- Apply the validated PEMFC 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 PEMFC model developed in this project can be employed to improve and optimize the design and operation of PEMFCs, 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.

## Fiscal Year (FY) 2011 Accomplishments

- Developed a 3-D, fully two-phase, single-cell model and completed the Year 2 model-development milestone, "Develop a 3-D, fully two-phase, single-cell PEM fuel cell model".
- Demonstrated the capabilities of the present fully two-phase single-cell model in case studies, including simulating a PEMFC with a complex Chevron flowfield.
- Made significant progress in model validation using polarization and current distribution data obtained by LANL using a *10*x*10* segmented cell.
- Developed and demonstrated a non-isothermal pore-network model for simulating water and thermal transport at the pore level.
- Performed 3-D computational fluid dynamics (CFD) simulation to verify the analytical droplet-detachment model developed previously.
- Carried out simplified calculations to estimate water flux at the gas diffusion layer (GDL)/channel interface.
- Investigated effect of cell segmenting on current-distribution measurements and developed guidelines on how a cell should be segmented to minimize the side effect of cell segmenting.
- Obtained current distribution maps experimentally using LANL's *10*x*10* segmented cell, and completed Year 2 experimental milestone, "Measure*10*x*10* current distribution performance data for model validation for four different operating conditions (relative humidity [RH] *=25%, 50%, 75%, 100%*)".
- "Polarization areas" with upper and lower bounds were obtained experimentally. Simultaneous current and temperature measurements were also obtained using mapping tool.

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## Introduction

As PEMFC 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 et al. [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, 3-D 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; it includes two other national laboratories (LANL and LBNL), 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 DAKOTA [2] (a software toolkit for design, optimization, and uncertainty quantification developed by SNL) 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 2011.

## 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 CFD 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. As mentioned previously, we have assembled a team of leading experts in PEMFC 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

Due to space limitation, only sample results are provided here. Figure 1 compares the partially two-phase model (in which flow in the channels is considered as single phase) with the fully two-phase model (in which flow in the channels is treated as two phase) by displaying along-channel contours computed by the two different models. Operating parameters are listed in Table 1, and detailed cell geometry and material (transport and physical) properties are provided in Table 1 of reference [1]. As expected, the partially two-phase model is not capable of capturing the two-phase behavior in the channels but the fully two-phase model does. Near the outlet of the cathode channel, liquid water is seen to be transported first from the channel to the GDL and then to the anode side due to drier anode inlet (note: counter flow is employed in the present work). In addition, the single-phase channel model predicts a dry-wet-dry transition pattern in the GDL-catalyst layer region whereas such wet-dry transition does not appear with the fully two-phase model since it predicts much more water in the channel.

Figure 2 shows liquid-saturation contours at the GFC (gas flow channel)/GDL interface as computed by the fully two-phase model for three anode/cathode inlet RH values: 42.5%, 66.4%, and 91.6%. Operating parameters are listed

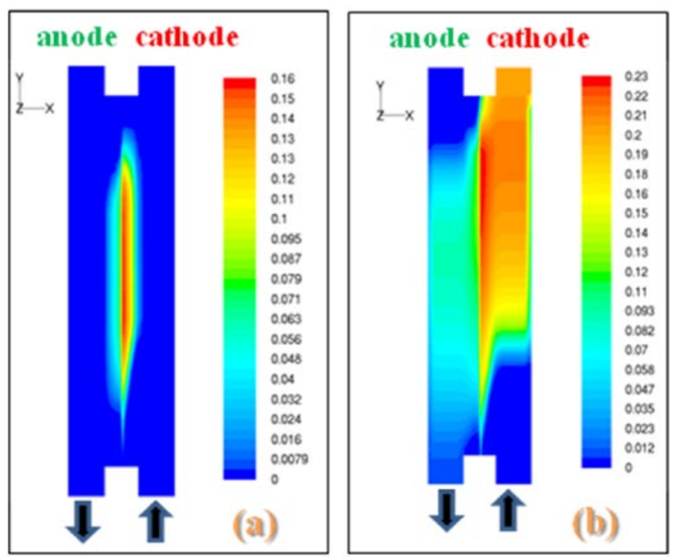


**FIGURE 1.** Partially two-phase model vs. fully two-phase model – computed liquid saturation contours on the symmetric plane: (a) partially two-phase model; and (b) fully two-phase model.

**TABLE 1.** Operating Conditions for the Base Case

| | | | |
|---|---|---|---|
| Current density | 0.8 A/cm$^2$ | Anode stoichiometric flow ratio | 1.8 |
| Cell temperature | 80°C | Cathode stoichiometric flow ratio | 2.0 |
| Anode/cathode back pressure | 200 kPa | Anode/cathode RH | 66.4% |

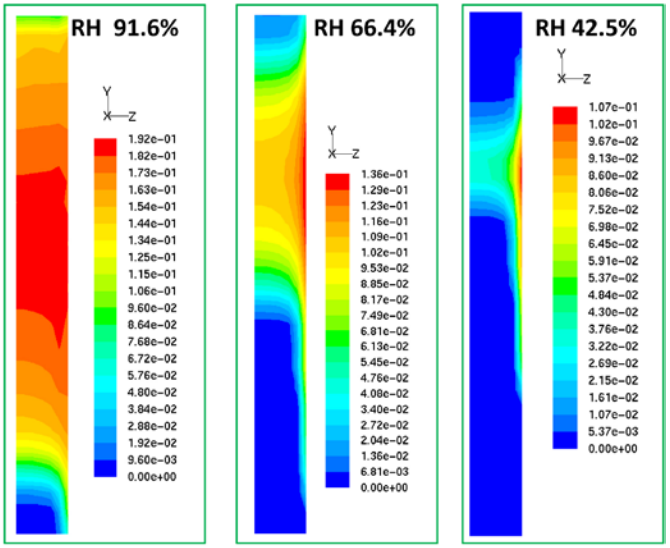


**FIGURE 2.** Computed liquid-saturation contours at the cathode GFC/GDL interface by the fully two-phase model – effect of inlet RH.

in Table 1. Clearly, more liquid water is accumulated in the cathode gas flow channel (GFC) as anode/cathode inlet RH is raised. Moreover, liquid saturation near the cathode outlet increases with increasing inlet RH, indicating that water transport from cathode to anode decreases.

Figure 3 displays computed liquid-saturation contours at the GFC/GDL interface for two current densities: 0.2 A/cm$^2$ and 1.5 A/cm$^2$. Operating parameters are listed in Table 1. It can be seen from Figure 3 that cathode GFC has more liquid water at low current densities than at high current densities – this most likely is due to that sufficiently large drag force is required to remove liquid water from the GFC. Of the four cases (0.1, 0.2, 1.0, and 1.5 A/cm$^2$) studied, cathode GFC has the most liquid water at current density of 0.2 A/cm$^2$. Lastly, as current density is reduced, it was found that the wet region in the cathode GFC enlarges gradually in both downstream and upstream, due to the smaller drag force of gas flow.

In Table 2, the current-density distribution computed using the fully two-phase model are compared with that measured using LANL's *10x10* segmented cell. The operating conditions are: 80°C, 50% RH, and 0.4 A/cm$^2$, and detailed cell geometry and material (transport and physical) properties are provided in Table 1 of reference [1]. From the numbers presented in Table 2, we can conclude that the agreement between computed and measured current density distribution is good with the root-mean-square error being less than 11.3% .

Lastly, a comparison between measured and computed polarization curves is presented in Figure 4, which shows good agreement. Geometric parameters, material (transport and physical) properties, and operating conditions for this study are presented in Table 1 of reference [1]. Further details on this model validation study is provided by Carnes et al. [3].

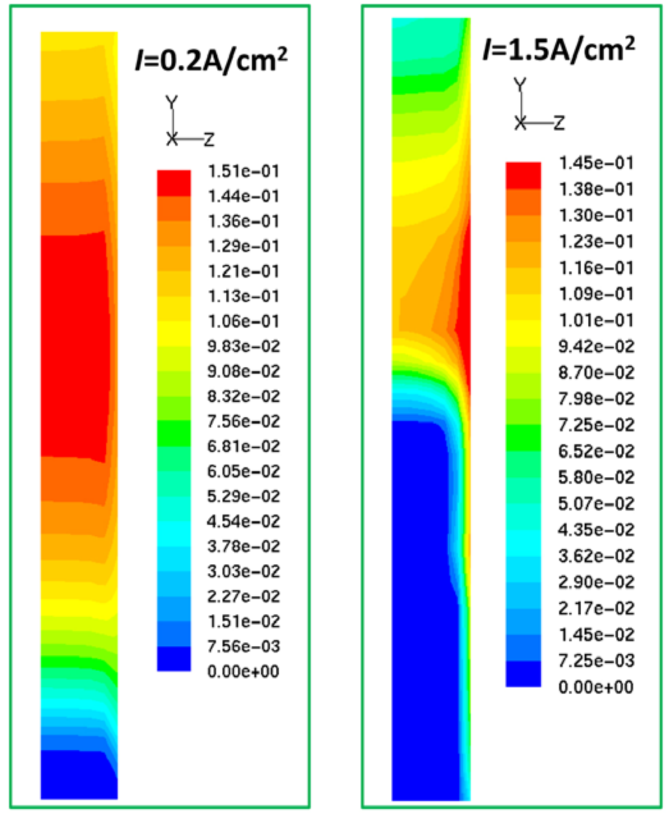


**FIGURE 3.** Computed liquid-saturation contours at the cathode GFC/GDL interface by the fully two-phase model – effect of current density.

**TABLE 2.** Computed vs. Measured Current-Density Distribution

**(a) Computed current-density distribution**

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0.31 | 0.36 | 0.37 | 0.37 | 0.37 | 0.37 | 0.38 | 0.38 | 0.39 | 0.34 |
| 0.33 | 0.39 | 0.39 | 0.39 | 0.39 | 0.39 | 0.39 | 0.39 | 0.39 | 0.34 |
| 0.35 | 0.41 | 0.41 | 0.41 | 0.40 | 0.40 | 0.40 | 0.39 | 0.39 | 0.33 |
| 0.33 | 0.40 | 0.41 | 0.41 | 0.42 | 0.42 | 0.42 | 0.42 | 0.43 | 0.36 |
| 0.36 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.42 | 0.36 |
| 0.36 | 0.44 | 0.44 | 0.44 | 0.43 | 0.43 | 0.43 | 0.43 | 0.42 | 0.36 |
| 0.34 | 0.42 | 0.42 | 0.43 | 0.43 | 0.43 | 0.44 | 0.44 | 0.44 | 0.37 |
| 0.36 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.42 | 0.42 | 0.42 | 0.35 |
| 0.35 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.41 | 0.41 | 0.35 |
| 0.31 | 0.37 | 0.37 | 0.38 | 0.38 | 0.39 | 0.39 | 0.39 | 0.39 | 0.34 |

**(b) Measured current-density distribution**

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0.00 | 0.43 | 0.39 | 0.38 | 0.38 | 0.38 | 0.38 | 0.37 | 0.37 | 0.37 |
| 0.36 | 0.41 | 0.40 | 0.41 | 0.41 | 0.41 | 0.41 | 0.40 | 0.39 | 0.39 |
| 0.39 | 0.43 | 0.44 | 0.46 | 0.45 | 0.46 | 0.45 | 0.45 | 0.42 | 0.42 |
| 0.41 | 0.46 | 0.46 | 0.45 | 0.48 | 0.50 | 0.50 | 0.48 | 0.45 | 0.45 |
| 0.41 | 0.48 | 0.49 | 0.47 | 0.46 | 0.51 | 0.53 | 0.53 | 0.49 | 0.48 |
| 0.41 | 0.45 | 0.47 | 0.47 | 0.46 | 0.49 | 0.51 | 0.49 | 0.48 | 0.49 |
| 0.40 | 0.43 | 0.47 | 0.47 | 0.48 | 0.47 | 0.46 | 0.46 | 0.43 | 0.45 |
| 0.37 | 0.44 | 0.44 | 0.46 | 0.45 | 0.46 | 0.45 | 0.44 | 0.43 | 0.44 |
| 0.37 | 0.38 | 0.40 | 0.41 | 0.42 | 0.44 | 0.43 | 0.43 | 0.45 | 0.40 |
| 0.35 | 0.36 | 0.31 | 0.28 | 0.38 | 0.36 | 0.37 | 0.38 | 0.31 | 0.00 |

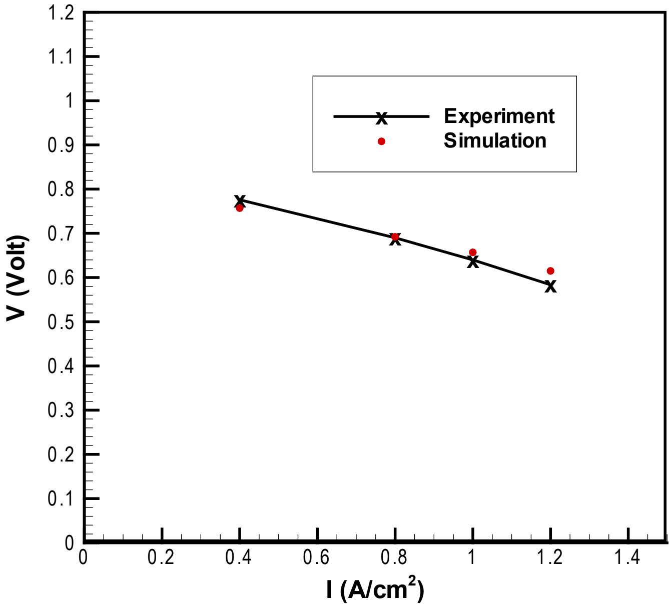


**FIGURE 4.** Model validation: comparison of measured and computed polarization curves.

## Summary and Conclusions

- A 3-D, fully two-phase, single-cell model for simulating PEMFC performance was developed and the milestone of developing a 3-D, fully two-phase, single-cell model was met.
- Significant progress has been made in model validation using polarization and current distribution data obtained by LANL using a *10*x*10* segmented cell.
- Current distribution maps were obtained experimentally using LANL's *10*x*10* segmented cell, and the Year 2 experimental milestone, "Measure*10*x*10* current distribution performance data for model validation for four different operating conditions (RH = *25%, 50%, 75%, 100%*) was met.

## Future Directions

- Complete model validation in the single-phase and partially two-phase regimes using LANL current-distribution data from segmented cell experiments, and test data from Ballard and Nissan.
- Complete sub-model and algorithm development, and numerical implementation.
- Develop a 3-D, two-phase, short-stack PEMFC model.
- Obtain water profiles in the through-plane using neutron radiography setup at the National Institute of Standard and Technology (NIST).
- Perform model validation in the fully two-phase regimes using neutron imaging data obtained by LANL at NIST, and test data from Nissan and Ballard.

## FY 2011 Publications/Presentations

**1.** Y. Wang and K.S. Chen, "Elucidating two-phase transport in a polymer electrolyte fuel cell, Part 1: Characterizing flow regimes with a dimensionless group", *Chemical Engineering Science*, **66**, 3557-3567 (2011).

**2.** Y. Wang, K.S. Chen, J. Mishler, S.C. Cho, X.C. Adroher, "A Review of Polymer Electrolyte Membrane Fuel Cells: Technology, Applications, and Needs on Fundamental Research", *Applied Energy*, **88**, 981-1007 (2011).

**3.** Y. Ji, G. Luo,a nd C.-Y. Wang, "Pore-level liquid water transport through composite diffusion media of PEMFC", *J. Electrochem. Soc.* **157** (12) B1753–B1761 (2010).

**4.** Y. Wang and K.S. Chen, "Through-plane water distribution in a polymer electrolyte fuel cell: comparison of numerical prediction with neutron radiography data", *J. Electrochem. Soc.*, **157** (12) B1878-B1886 (2010).

**5.** Y. Wang and K.S. Chen, "Elucidating through-plane Liquid Water Profile in a Polymer Electrolyte Fuel Cell", in *ECS Transaction*, **33**(1) 1605-1614 (2010).

**6.** K.S. Chen, B. Carnes, L. Hao, Y. Ji, G. Luo, C.-Y. Wang, and Y. Wang, "Toward the development and validation of a comprehensive PEM fuel cell model," in *ASME Proceedings of ESFuelCell2011*, paper #54693; and also presentation in the 9th Int. Fuel Cell Science, Engineering & Technology Conference, Aug. 7–10, 2011, Washington, DC.

**7.** B. Carnes, K.S. Chen, L. Hao, G. Luo, Y. Ji, C.-Y. Wang, and D. Spernjak, "Validation and uncertainty quantification of a two-phase, multidimensional PEMFC computer model using high-resolution segmented current collector data," in *ASME Proceedings of ESFuelCell2011*, paper #54746; and also presentation in the 9th Int. Fuel Cell Science, Engineering & Technology Conference, August 7–10, 2011, Washington, D.C.

**8.** K.S. Chen, "Development and validation of a three-dimensional, two-phase, PEM fuel cell model", presentation at the *2011 DOE Hydrogen Program Annual Merit Review and Peer Evaluation Meeting*, Washington DC, May 9–13, 2011, paper #FC027.

**9.** K.S. Chen, "Development and Validation of a Two-phase, Three-dimensional Model for PEM Fuel Cells", invited presentation at the 2010 LANL(US)/AIST-NEDO(Japan) Fuel Cell Workshop, Hyatt Regency Waikiki Beach Resort, Honolulu, HI, Aug 9–11, 2010.

## Reference

**1.** K.S. Chen, B. Carnes, L. Hao, Y. Ji, G. Luo, C.-Y. Wang, and Y. Wang, "Toward the development and validation of a comprehensive PEM fuel cell model," in *ASME Proceedings of ESFuelCell2011*, paper #54693 (2011).

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

**3.** B. Carnes, K.S. Chen, L. Hao, G. Luo, Y. Ji, C.-Y. Wang, and D. Spernjak, "Validation and uncertainty quantification of a two-phase, multidimensional PEMFC computer model using high-resolution segmented current collector data," in *ASME Proceedings of ESFuelCell2011*, paper #54746 (2011).