SANDIA NATIONAL LABORATORIES
FUEL CELLS R&D PROJECT

QUARTERLY PROGRESS REPORT FOR OCTOBER 1, 2010–DECEMBER 31, 2010

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RECIPIENT: SANDIA NATIONAL LABORATORIES

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PROJECT TITLE:	DEVELOPMENT AND VALIDATION OF A TWO-PHASE, THREE-DIMENSIONAL MODEL FOR PEM FUEL CELLS
COVERING PERIOD:	OCTOBER1, 2010 THROUGH DECEMBER 31, 2010
DATE OF REPORT:	JANUARY 10, 2011
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OTHER KEY NATIONAL LAB RESEARCHERS:	BRIAN CARNES (SNL)
SUBCONTRACTORS FUNDED THROUGH AOP TASK:	PENN STATE UNIV., BALLARD POWER SYSTEMS
INDUSTRIAL PARTNERS:	NONE
DOE MANAGERS:	JASON MARCINKOSKI, DONNA HO

INTRODUCTION

PROJECT OBJECTIVE

The objectives of this project are twofold: (1) to develop and validate a two-phase, three-dimensional transport model for simulating polymer electrolyte membrane (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.

BACKGROUND

Despite tremendous research efforts and a large number of models published in the literature, 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. Modeling PEM fuel cell operation is challenging because it involves 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, along with relatively high inlet relative humidity or moderate cell temperature, further add to the modeling challenges.

In this project, we shall employ a combined computational and experimental approach. First, we'll develop a two-phase, three-dimensional, transport model for simulating PEM fuel cell performance under a wide range of operating conditions. Next, we'll validate our transport

model in a staged approach using experimental data available from the literature and those generated by team members. Lastly, we'll apply the validated model to identify performance-limiting phenomena or processes and develop recommendations for improvements. The major task in this proposal is the development of the PEM fuel cell transport model, which requires input parameters and validation. Once the model is validated, we shall apply it to identify performance-limiting phenomena or processes and develop recommendations for improvements. As required by DOE, we shall also publically disseminate and document the model, and compile data generated. Consequently, at a high level there are five tasks in this project:

1. Develop a two-phase, three-dimensional, PEM fuel cell transport model;

2. Measure model-input parameters and generate model-validation data;

3. Validate the two-phase, three-dimensional PEM fuel cell transport model;

4. Identify performance-limiting phenomena or processes and develop recommendations for improvements; and

5. Disseminate/document the models developed and compile data generated.

DEVELOPMENT AND VALIDATION OF A TWO-PHASE, THREE-DIMENSIONAL MODEL FOR PEM FUEL CELLS

PROJECT STATUS

The following were accomplished/carried out during this quarter:

1. Efforts were initiated to develop a first-generation, 3-D, fully two-phase, single-cell PEM fuel cell model; specifically, we are making progress in implementing a sub-model for simulating two-phase flow in the gas channels and investigating the associated numerical issues.

2. We are also making progress on computationally justifying the current distribution measurement technique by segmenting bipolar plates. Preliminary results show that segmented cell is an intrusive technique and without proper guidelines, the accuracy for measuring the current distribution in the membrane can be unacceptable.

3. Efforts were also initiated to perform validation of the 3-D, partially two-phase, single-cell PEM fuel cell model developed previously in Year 1. Specifically, we further improved the partially two-phase PEM fuel cell model to make it more suitable for large-scale simulation. A large-scale mesh (with an active area of 50 cm^2) having one million cells was generated to test the parallel computation capability.

4. We are improving the pore-network model developed previously by including two-way coupling between pore-level liquid water transport and continuum-level heat transfer and incorporating additional effects, such as liquid water imbibitions, pore-level vapor diffusion and evaporation in the model.

5. Tests for obtaining model validation data for the single-phase regime (in which liquid water effects are negligible), including the O_2 sensitivity test on a 10-cell stack, were completed by Ballard and documented.

On December 6, 2010, we held a project review at the DOE Headquarters in which team partners (SNL, PSU, LANL, LBNL, Ballard) made respective progress-report presentations. Patricia Chong of Ballard also made a presentation on end-user/customer expectations. Brian Carnes of SNL conducted a live demo of the PEM fuel cell model and its coupling with DAKOTA (a design and optimization toolkit developed by SNL) that is being developed by the SNL-PSU subteam. This project review was hosted by Jason Marcinkoski and attended by others (Dimitrios Papageorgopoulos, Nancy Garland, Kathi Epping Martin, Donna Ho) in the Fuel Cell Team at DOE as well as Technical Advisor, Walt Podolski of ANL.

PLANS FOR NEXT QUARTER AND KEY ISSUES

1. Complete the development of a first-generation, 3-D, fully two-phase, single-cell PEM fuel cell model; and

2. Continue to work on and make significant progress toward validating the 3-D, partially two-phase, single-cell PEM fuel cell model developed previously in Year 1.

PATENTS

None

PUBLICATIONS/PRESENTATIONS

1. K. S. Chen, B. Carnes, L. Hao, Y. Ji, G. Luo, C.-Y. Wang, and Y. Wang, "Toward the development and validation a comprehensive PEM fuel cell model," abstract accepted for presentation at the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

2. B. Carnes, K. S. Chen, L. Hao, G. Luo, Y. Ji, and C.-Y. Wang, "Validation and uncertainty quantification of a two-phase, multidimensional PEMFC computer model using high-resolution segmented current collector data," abstract accepted for presentation at the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

3. G. Luo, L. Hao, Y. Ji, C.-Y. Wang, B. Carnes, and K. S. Chen, "Computational justification of current distribution measurement technique by segmenting bipolar plate,"

abstract accepted for presentation at the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

4. L. Hao, G. Luo, Y. Ji, C.-Y. Wang, B. Carnes, and K. S. Chen, "Fully two-phase modeling for PEM fuel cells," abstract accepted for presentation at the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

5. Y. Wang and K. S. Chen, "Modeling effects of two-phase transport in cathode gas flow channel on PEM fuel cell performance," abstract accepted for presentation at the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

6. Y. Ji, G. Luo, and C.Y. Wang, "Pore network modeling of two-phase transport in GDL with heat transfer and phase change," abstract accepted for presentation at the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

PROJECT TITLE:	ANION EXCHANGE MEMBRANE FUEL CELL
COVERING PERIOD:	SEPTEMBER, 2010 TO JANUARY 30, 2011
DATE OF REPORT:	JANUARY 5, 2011
PRINCIPLE INVESTIGATOR:	CY FUJIMOTO, (505) 844-6432, CHFUJIM@SANDIA.GOV
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SUBCONTRACTORS FUNDED THROUGH AOP TASK:	NONE
DOE MANAGER:	JASON MARCINKOSKI

ANION EXCHANGE MEMBRANE FUEL CELL

PROJECT STATUS

In our previous report, we discussed good alkaline fuel cell performance using the Sandia material [Diels-Alder poly(phenylene)] with benzyltrimethyl ammonium cation groups attached (Figure 1). The cell used in Figure 1 was operated at 60 °C with H_2/O_2 and Pt black (4 mg/cm^2) on each electrode. At high voltages, 0.8 V, the output current density is near 100 mA/cm^2 and at 0.4 V the output current density is near 300mA/cm^2.

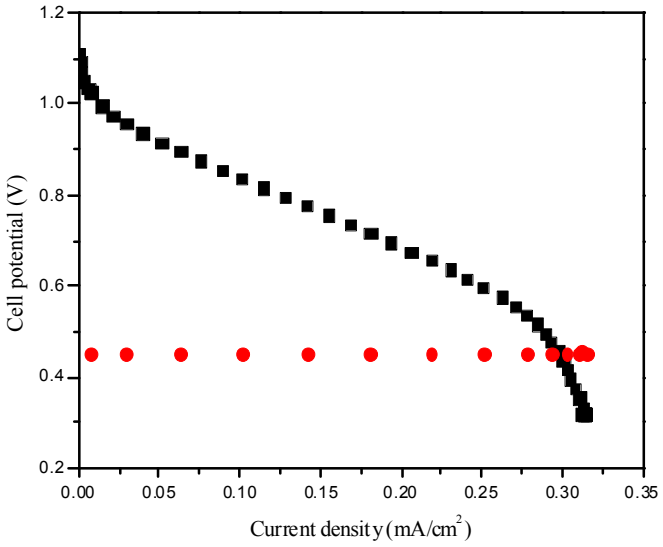

Figure 1. Best alkaline fuel cell performance from previous quarter, operated at 60 °C.

Since our last report we have prepared, characterized and sent several films for MEA fabrication and further testing by our partners at LANL. Figure 2 displays the most recent fuel cell performance taken by our partners at LANL using the Sandia material [IEC: 1.82eq/g, water uptake: 47%, hydroxyl conductivity: 57mS/cm at RT]. In this polarization curve we see improvements in performance under both high and low voltages; 0.8-V output current is near 150 mA/cm^2 and at 0.4 V the output current is near 450 mA/cm^2. As expected, when the temperature is raised from 60 °C to 80 °C, the high-frequency resistance drops slightly and the cell performance is further enhanced (Figure 3).

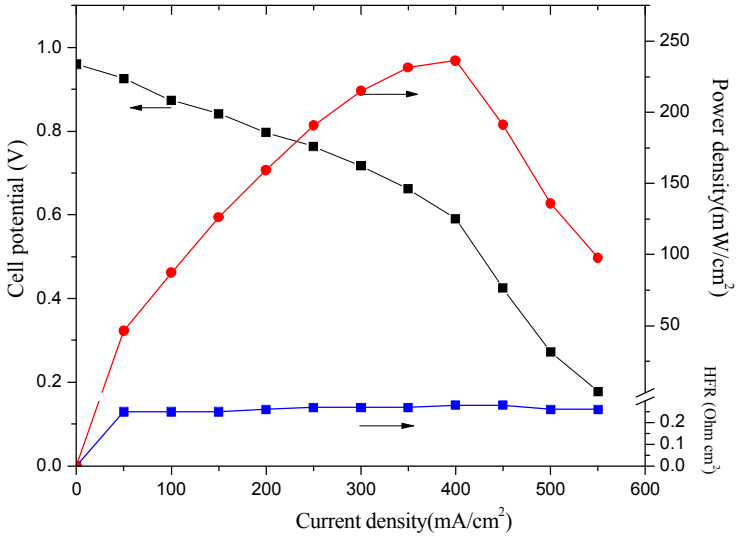

Figure 2. Current alkaline fuel cell performance at 60 °C.

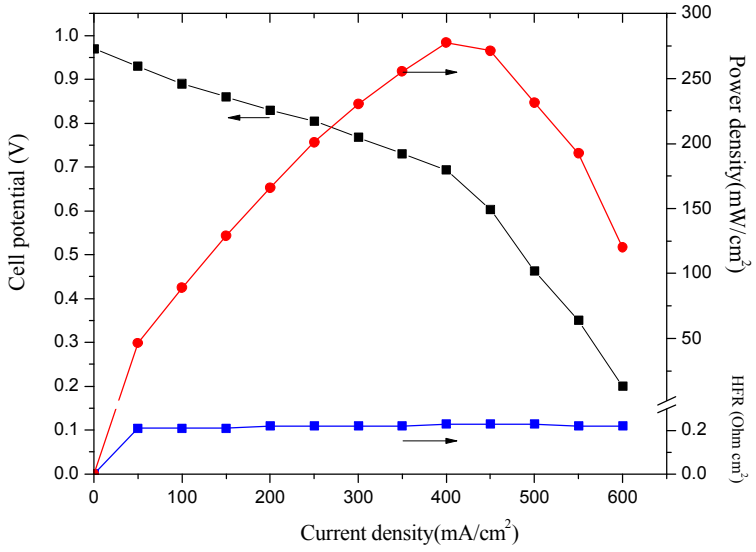

Figure 3. Current alkaline fuel cell performance at 80 °C.

One of the challenges that we are currently facing however, is film brittleness. Through this work we have been observing that most of the alkaline films are difficult to handle, especially when the films are dry. This makes MEA fabrication very difficult and raises concerns regarding fuel cell durability issues. We have been working to resolve this issue through polymer blending. In Figure 4, we blended the Sandia material with an elastomer. Stress-strain curves were taken of the pristine Sandia material (sample A) with varying degrees of the elastomeric additive (ranging from 1–5% by weight). As can been seen, thus far all of the blends had poorer mechanical properties than the pure Sandia material.

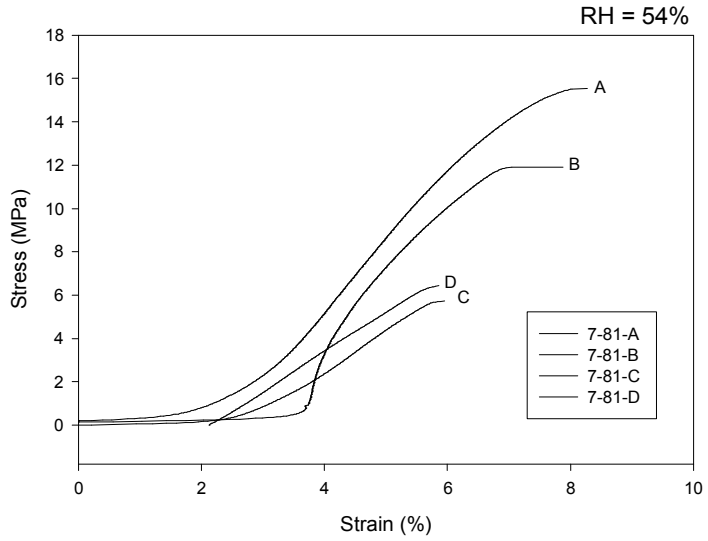

Figure 4. Stress-strain curves of Sandia material with varying degrees of elastomer additive.

PLANS FOR NEXT QUARTER

In the upcoming quarter we plan to continue improving the mechanical properties of the membranes by blending with other elastomers to reduce brittleness. We also plan to continue sending samples to our partners at LANL so further optimization of MEA fabrication and alkaline fuel cell performance can be achieved.

PATENTS

None

PUBLICATIONS/PRESENTATIONS

M. R. Hibbs, "Recent advances in anion exchange membranes for alkaline fuel cells," invited presentation at the 2010 NEDO-LANL Fuel Cell Workshop, Hyatt Regency Waikiki Beach Resort and Spa, Honolulu, HI, August 9–11, 2010.