SAND2011-3154P
SAND2011-XXXX P

SANDIA NATIONAL LABORATORIES
FUEL CELLS R&D PROJECT

QUARTERLY PROGRESS REPORT FOR JANUARY 1, 2011–MARCH 31, 2011

SUBMITTED BY: JAY KELLER, (925) 294-3316, JOKELLE@SANDIA.GOV

RECIPIENT: SANDIA NATIONAL LABORATORIES

CONTENTS

DEVELOPMENT AND VALIDATION OF A TWO-PHASE, THREE-DIMENSIONAL MODEL FOR PEM FUEL CELLS 2
PROJECT OBJECTIVE 2
BACKGROUND 2
PROJECT STATUS 3
PLANS FOR NEXT QUARTER AND KEY ISSUES 4
PATENTS 4
PUBLICATIONS/PRESENTATIONS 4
ANION EXCHANGE MEMBRANE FUEL CELL 5
PROJECT STATUS 5
PLANS FOR NEXT QUARTER 7
PATENTS 7

PROJECT TITLE:	DEVELOPMENT AND VALIDATION OF A TWO-PHASE, THREE-DIMENSIONAL MODEL FOR PEM FUEL CELLS
COVERING PERIOD:	JANUARY 1, 2011 THROUGH MARCH 31, 2011
DATE OF REPORT:	APRIL 25, 2011
PRINCIPLE INVESTIGATOR:	KEN S. CHEN, 505-844-5783, KSCHEN@SANDIA.GOV
OTHER KEY NATIONAL LAB RESEARCHERS:	BRIAN CARNES (SNL)
SUBCONTRACTORS FUNDED THROUGH AOP TASK:	PENN STATE UNIV., UC IRVINE, BALLARD POWER SYSTEMS
INDUSTRIAL PARTNERS:	NISSIAN MOTOR CO., LTD
DOE MANAGERS:	DONNA HO, JASON MARCINKOSKI

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

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.

PROJECT STATUS

The following were accomplished/carried out during this quarter:

1. A first-generation, three-dimensional, fully two-phase, single-cell PEM fuel cell model was developed and demonstrated in parametric studies.

2. The first-generation, 3-D, fully two-phase, single-cell PEM fuel cell model was further demonstrated by employing it to simulate a PEM fuel cell with a Chevron flowfield.

3. Significant progress was made toward validating the partially two-phase, single-cell PEM fuel cell model developed in FY10, using polarization and current distribution data obtained by Las Alamos National Lab using a 10 x 10 segmented cell.

4. A non-isothermal pore network model was developed and demonstrated.

5. Three-dimensional CFD (Computational Fluid Dynamics) simulation was performed to verify the analytical model for water-droplet detachment.

6. A project team meeting was held on March 4 via teleconference in which team members or project partners provided technical progress updates. We also discussed the preparation for the 2011 Annual Merit Review meeting to be held on May 9–13, 2011 in Washington, D.C.

PLANS FOR NEXT QUARTER AND KEY ISSUES

1. Complete Milestone 3, "Develop a 3-D, fully two-phase, single-cell model and demonstrate model utility in case studies with acceptable numerical convergence measured by absolute residual of 10^{-5} or less and mass/charge balance error of 2% or less."

2. Make significant progress toward completing Milestone 5, "Perform validation of the 3-D, partially two-phase, single-cell model by comparing computed and measured polarization curves, and current distributions with reasonable agreement (errors fall into the 99% confidence interval or within +/- 15%)."

PATENTS

None

PUBLICATIONS/PRESENTATIONS

1. 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).

2. 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).

3. 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).

4. 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," draft proceeding paper submitted for publication in Proceedings of the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

5. 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," draft proceeding paper submitted for publication in Proceedings of the ASME 9th International Fuel Cell Science, Engineering and Technology Conference to be held in Washington, D.C., August 7–10, 2011.

ANION EXCHANGE MEMBRANE FUEL CELL

PROJECT TITLE:	ANION EXCHANGE MEMBRANE FUEL CELL
COVERING PERIOD:	JANUARY 30, 2011 TO APRIL 30, 2011
DATE OF REPORT:	JANUARY 5, 2011
PRINCIPLE INVESTIGATOR:	CY FUJIMOTO, (505) 844-6432, CHFUJIM@SANDIA.GOV
OTHER KEY NATIONAL LAB RESEARCHERS:	NIGEL SAMMES, (505) 284-4337, NMSAMME@SANDIA.GOV JAY KELLER, (925) 294-3316, JOKELLE@SANDIA.GOV
SUBCONTRACTORS FUNDED THROUGH AOP TASK:	NONE
DOE MANAGER:	JASON MARCINKOSKI

PROJECT STATUS

In this past quarter, in collaboration with LANL, we were able to definitively determine that poly(phenylene)s materials that we have been developing at Sandia are chemically more stable than the typically studied poly(arylene) ether structure in an alkaline fuel cell environment. Our collaborators at LANL synthesized two different poly(arylene) ethers [Figure 1]. However, they found that during the base soak, both an increase in base concentration and the amount of time of the base soak severely reduced the mechanical property of these films [Figure 1].

The reduction in mechanical strength of the films is attributed to nucelophilic attack of the hydroxyl anion to the polymer backbone to the ether linkage. When these same studies were conducted using our poly(phenylene)s, there were no change in the mechanical properties after base soak; varying concentration, temperature and time [Figure 2].

Finally, further improvements were made in alkaline fuel cell performance. Team members at LANL have developed a new electrode binder to reduce the resistive interface between the polymer membrane and the electrode. In Figure 3 the red and green traces are data taken using previous binder material (aminated TMPP) which showed drops in performance possibly due to flooding and high interfacial resistance. However, with the newly developed binders by LANL, in combination with the aminated TMPP, we observe lower interfacial resistance, better mass transport, and maximum power densities of 236 mW/cm^2 (at 60 ^oC) and 278 mW/cm^2 (at 80 ^oC).

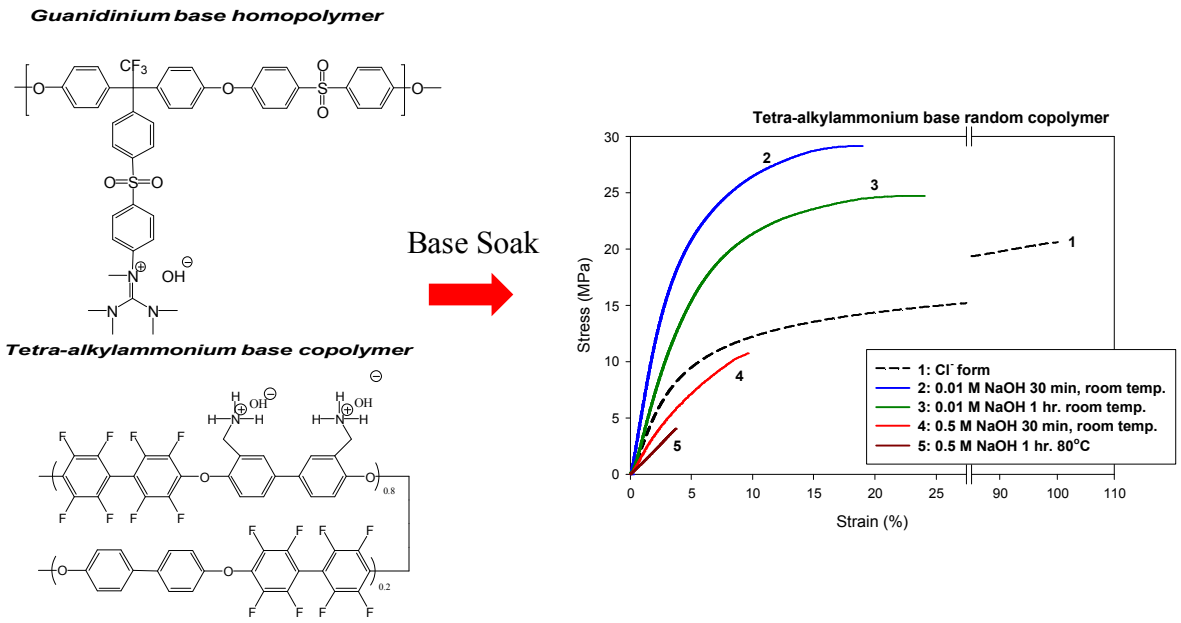

Figure 1. Reduced mechanical property of poly(arylene) ether backbone after soaking in NaOH.

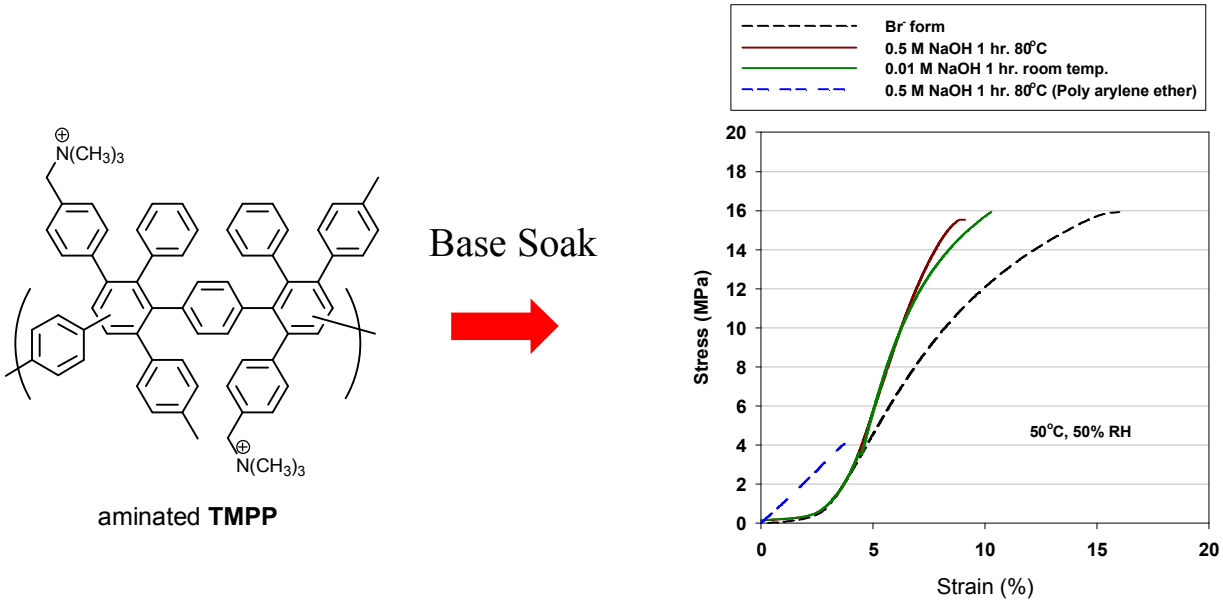

Figure 2. Mechanically stable ATMPP under various NaOH concentration and temperature.

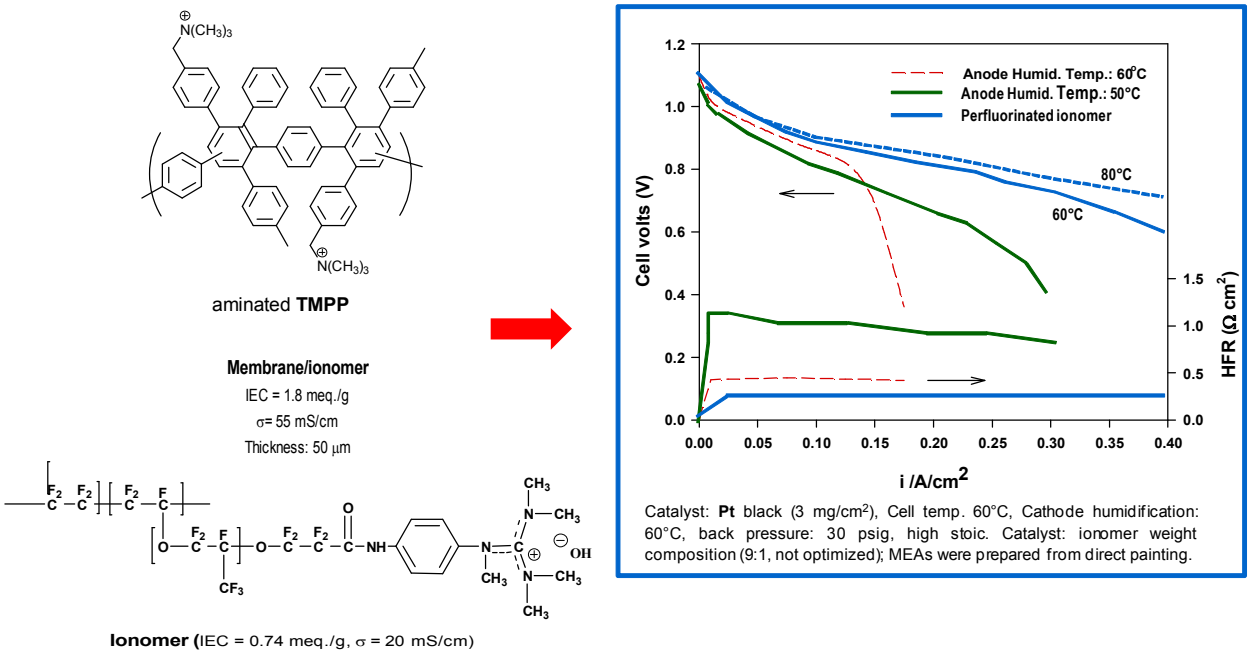

Figure 3. Alkaline fuel cell performance with different binders ATMPP (red and green) vs. perfluoronated (blue) under H_2/O_2.

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