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Quarterly Progress Report

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Project Title: Hydrogen PEMFC Water Transport, B&R # EB4209, EEW112798.

Project Period: January 1, 2008 to March 31, 2008
Date of Report: April 7, 2008

Principle Investigator: Ken S. Chen, 505-844-5783, kschen@sandia.gov
Other Key National Lab Researchers:

Sub-Contractors Funded through AOP Task: Chao-Yang Wang, Penn State Univ.

Industrial Partners: none

DOE Managers: Nancy Garland

Project Objective: To develop analytical and multi-dimensional models for simulating (1) water transport and removal in a PEM (proton exchange membrane or polymer electrolyte membrane) fuel cell under normal operation conditions, (2) ice formation after the shut down of a PEM fuel cell under freezing conditions, and (3) thawing during start-up from frozen conditions in a PEM fuel cell.

Background: Particularly during peak power conditions, water generated in the oxygen reduction reaction and transported from anode to cathode via electro-osmotic drag must be removed efficiently in order to achieve and maintain high PEM (proton exchange membrane or polymer electrolyte membrane) fuel cell performance. Under freezing conditions, residual water within a PEM fuel cell after its shut-down can freeze. The formation of ice within MEA (membrane electrode assembly) can hinder reactant transport, cause mechanical stresses to develop, and degrade cell voltage. Ice formed after the shutdown of a PEM fuel cell must be thawed during its start-up for given frozen conditions.

In this sub-project, we propose to develop analytical and multi-dimensional models for simulating 1) water transport and removal under normal operation conditions; 2) ice formation after the shut down of a PEM fuel cell under freezing conditions; and 3) thawing during start-up from frozen conditions in a PEM fuel cell. Specifically, we propose to develop sub-models for liquid water removal via droplet detachment and evaporation. Furthermore, we propose to develop multi-dimensional models for simulating water transport and removal under normal operating conditions, ice formation under freezing conditions, and thawing during start-up from frozen conditions.

Status: A first-generation three-dimensional (3-D) numerical model was developed to simulate water-droplet detachment from the interface between the gas diffusion layer and gas flow channel. The 3-D droplet-detachment numerical model was documented in a draft paper that was accepted for presentation at the *6th International Fuel Cell Science, Engineering & Technology Conference* to be held in Denver, Colorado, June 16 – 18, 2008 and for publication in the ASME *FUELCELL08 Proceedings.* We are in the process of improving, verifying, and validating the 3-D droplet-detachment numerical model. During this quarter, the PI has also participated in the US-Canada Fuel Cell Workshop held in the Institute for Fuel Cell Innovations, National Research Council of Canada, Vancouver, Canada, March 17 – 18, 2008.

Plans for Next Quarter and Key Issues: Complete the development, verification, and validation of the 3-D droplet-detachment model and demonstrate its utility in case studies. Continue the development of a sub-model for analyzing liquid-water removal via evaporation.

Patents: none.

Publications:

1. K. S. Chen and M. A. Hickner, "Elucidating water transport and removal in PEM fuel cells via experiments and modeling", paper presented at the *US-Canada Fuel Cell Workshop* held at the *Institute for Fuel Cell Innovations*, *National Research Council*, Vancouver, Canada, March 17 – 18, 2008.
2. K. S. Chen, "Modeling Water-Droplet Detachment from GDL/Channel Interfaces in PEM Fuel Cells", draft paper accepted for presentation at the *6th International Fuel Cell Science, Engineering & Technology Conference* to be held in Denver, Colorado, June 16 – 18, 2008 and for publication in the ASME *FUELCELL08 Proceedings*.