Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization

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Prepared for:
DOE Hydrogen Fuel Cell Kickoff Meeting

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Background

Water Management Issues Arise From:

- Generation of water by cathodic reaction
- Membrane humidification requirements
- Capillary pressure driven transport through porous MEA and GDL materials
- Scaling bipolar plate channel dimensions

Relevant Barriers and Targets

- Improved Gas Diffusion Layer, Flow Fields, Membrane Electrode Assemblies Needed to Improve Water Management:
  - Flooding blocks reactant transport
  - Drying out of membrane reduces protonic conductivity
  - Water distribution at shutdown, and transport during start-up, affects transient response, cold-start capability, and materials requirements for freeze-thaw cycle robustness

- Water management improvements are needed to maintain advances in transient response and cold start-up time, while improving power performance (650 W/L power density by 2010)
Program Objectives

- Develop advanced physical models and conduct material and cell characterization experiments to improve and optimize fuel cell design and operation;

- Demonstrate improvements in water management resulting in improved efficiency during automotive drive cycles, freeze/thaw cycle tolerance, and faster cold startup;

- Improve understanding of the effect of various cell component properties and structure on the gas and water transport in a PEM fuel cell, particularly the gas diffusion media (GDM) and flow channels; and

- Encapsulate the developed models in a commercial modeling and analysis tool, allowing transfer of technology to the industry for future applications.
Approach

Overall:
- Integrated experimental characterization and model development
- Systematically address each of the component regions of the cell
- Integrate the developed advanced modeling capabilities into an analysis tool capable of addressing water transport issues in future generation cell designs

Modeling Approach:
- Develop advanced models for water transport, and model parameters, in cell component materials
- Evaluate, and verify the developed models and parameters in a CFD based simulation tool for unit cell performance simulation
- Apply verified modeling capabilities and simulation results to devise and screen cell and stack performance improvement approaches

Experimental Approach:
- Perform ex-situ materials characterization to support and guide model development
- Gather in-situ diagnostics for model test and verification
- Characterize cell flooding sensitivity to materials and operating strategies
- Implement and test performance improvement strategies
CFDRC Prior Work: Example Case

- 50 cm² fuel cell with 4 serpentine channels
- Three-dimensional model, ~1.4 million grid cells

**Cell Dimensions:**
Length and Width ~ 6.9 cm

**Dimensions of various layers:**
- Diffusion Layer ~ 230 microns
- Catalyst Layer ~ 20 microns
- Membrane ~ 50 microns
- Channel depth ~ 1.016 mm
- Channel width ~ 0.7874 mm
CFDRC Prior Work: Sample Results

- Operating conditions: 100% relative humidity, 80°C, 1 atm pressure, $V_{cell} = 0.225$ V
- Distributions of current density (membrane mid-section) and liquid water saturation (cathode catalyst layer midsection):

High Inlet Humidity at Low Cell Voltages Results in Larger Quantities of Liquid Saturation and Cell Flooding
Model Testing at Ballard

Independent comparison to cell diagnostic data:

- High current prediction is adequate on average, but local current distribution errors are high.
- Predictions are poor at low current densities (needed for automotive drive cycles) and are the subject of ongoing improvement.
- Breakdown of MEA water into GDLs and membrane is not accurate.
- Modeling and design of the MEA water distribution is critical to cell durability and freeze start capability.
## Work Schedule and Milestones

### Estimated Start Date: April 1, 2007

- **Ex-Situ Characterization:**
  - Baseline material properties

- **Cell and Stack Characterization**
  - Initial data delivery

- **Model Development:**
  - Physical models down-selected and implemented
  - LBM coded and ready for test

- **Model Test/Validate**
  - Single and Multi-Component LBM
  - Establish confidence levels for application / need for model and parameter improvements / optional models

- **Optimization and Demonstration**
  - Deliver demonstration Stack

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<th>TASK DESCRIPTION</th>
<th>Year 1</th>
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Key Decision Points

- **Cell Scale Model Development:**
  - FY07 Q3 (Jun 2007): Down-select basic transport model formulation
  - FY09 Q1 (Dec 2008): Go/NoGo Decision for improving/extending membrane water transport and electrochemical kinetics based on outcome of steady-state and initial transient testing

- **LBM Model Development:**
  - FY08 Q2 (Mar 2008): Go/NoGo for continued development and extension to multi-component
  - FY08 Q4 (Sep 2008): Go/NoGo for continued activity (begin application)

- **Design/Operational/Materials Improvement:**
  - FY09 Q2 (Mar 2009): Select (3) candidate strategies for additional screening via simulation and additional experiments
## Budget Summary

By Fiscal Year:

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- Total Budget $6.03M,
- DOE Funding $4.7M,
- 22% of costs shared by team
Corporate Overview

*Multi-Disciplinary Engineering Solutions*

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- Better Insights
- Better Decisions for:
  - New Designs
  - Concepts
  - Operations
  - Safety

Simulations & Experiments

- Innovative Designs & Prototypes
- Better Products with:
  - Greater Functionality
  - Reduced Costs
  - Shorter Time to Market
  - Lower Risk

Better Decisions, Better Products
Through Simulation & Innovation

Specializing in Engineering Simulation, Design, Analysis, Prototyping and Systems Applications
Track Record

CFDRC REVENUE ($M)

QUALIFIED PERSONNEL

PhD 55%
MSC 20%
Other 25%

Over 25 Patents (For Licensing and Customization)

Metered Dose Inhaler Spacer
Synthetic Microvascular Networks
Constant Volume Rocket Motor
High Energy Hypergolic Bipropellant Gels

Dielectrophoresis Cell Sorter
Electrostatic Air Sampler
Thrombectomy Catheter
Microfluidic Mixing and Cleaning

Specializing in Engineering Simulation, Design, Analysis, Prototyping and Systems Applications